Faculty of Physics

WARSAW UNIVERSITY OF TECHNOLOGY

ALICE

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Using Machine Learning for Particle Identification in ALICE

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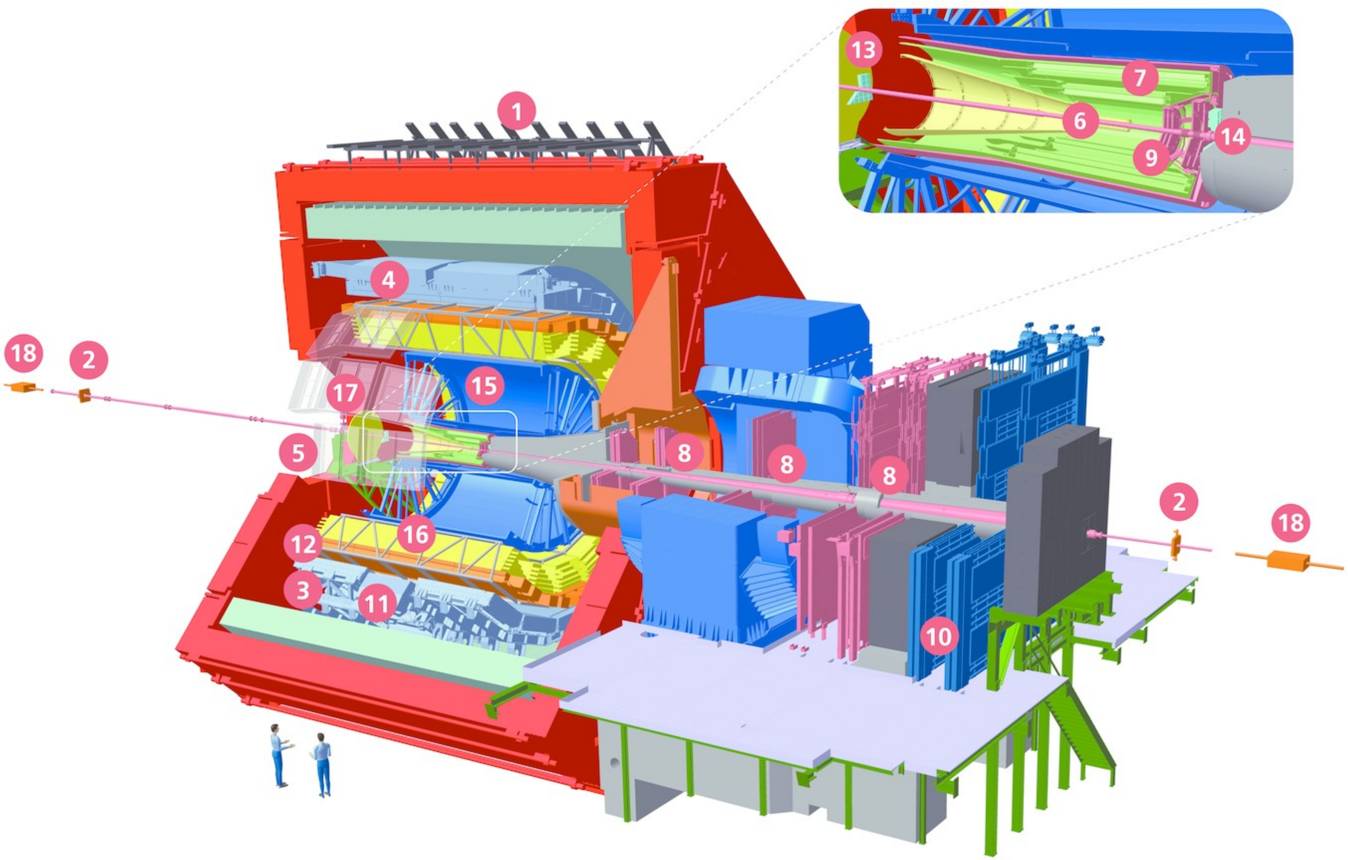
for the ALICE Collaboration

AI4EIC-Exp Workshop

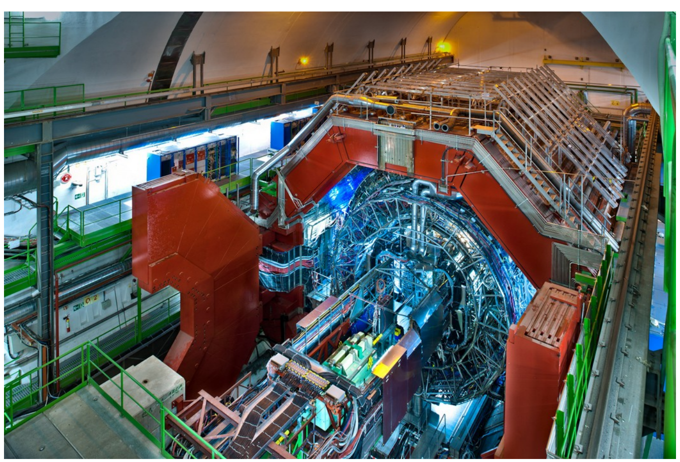
BNL, USA

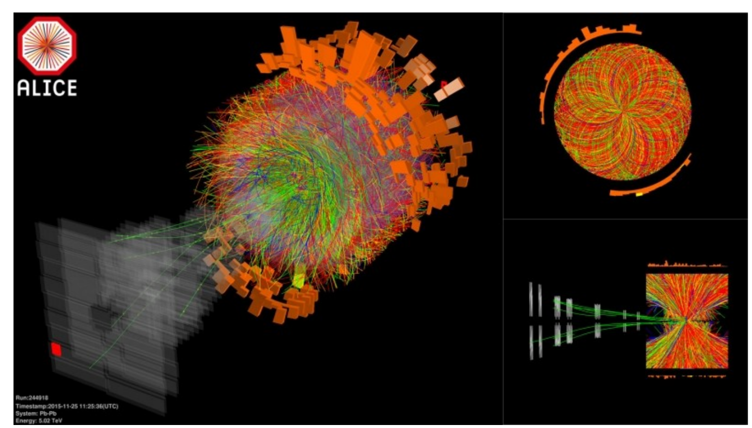
8/09/2021

The ALICE experiment



1. **ACORDE** | ALICE Cosmic Rays Detector
2. **AD** | ALICE Diffractive Detector
3. **DCal** | Di-jet Calorimeter
4. **EMCal** | Electromagnetic Calorimeter
5. **HMPID** | High Momentum Particle Identification Detector
6. **ITS-IB** | Inner Tracking System - Inner Barrel
7. **ITS-OB** | Inner Tracking System - Outer Barrel
8. **MCH** | Muon Tracking Chambers
9. **MFT** | Muon Forward Tracker
10. **MID** | Muon Identifier
11. **PHOS / CPV** | Photon Spectrometer
12. **TOF** | Time Of Flight
13. **T0+A** | Tzero + A
14. **T0+C** | Tzero + C
15. **TPC** | Time Projection Chamber
16. **TRD** | Transition Radiation Detector
17. **V0+** | Vzero + Detector
18. **ZDC** | Zero Degree Calorimeter





Goals of the WUT team

- Use ALICE and its data as a unique environment to advance the Machine Learning field of science
- Identify areas where both ALICE (or HEP in general) and ML communities can mutually benefit
- More focus on Machine Learning research rather than using standard ML tools for ALICE use cases

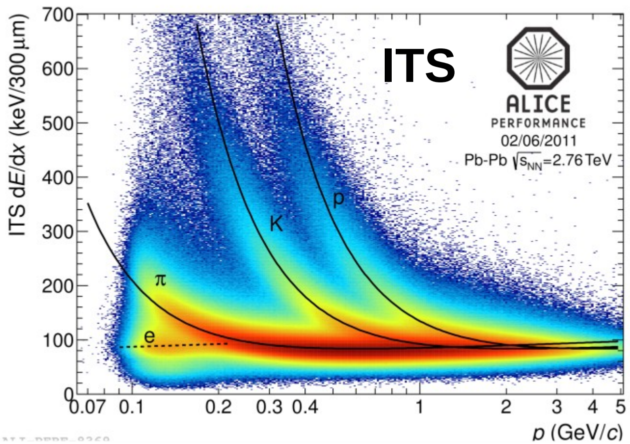
- Disclaimer:
  - I'm a physicist working with ML experts from the WUT IT department
  - My task is to guide and coordinate the work of WUT ML computer scientists within ALICE

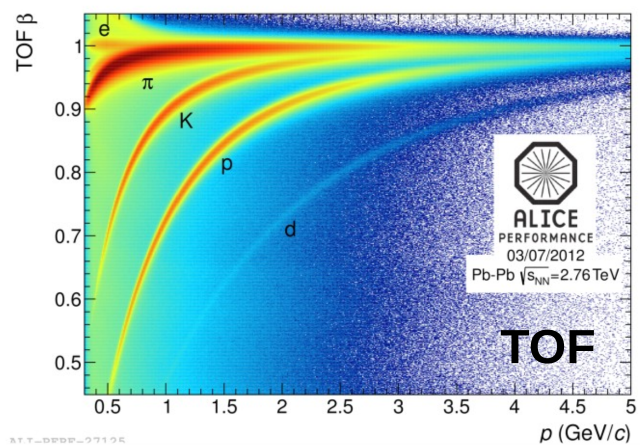
PID with Machine Learning

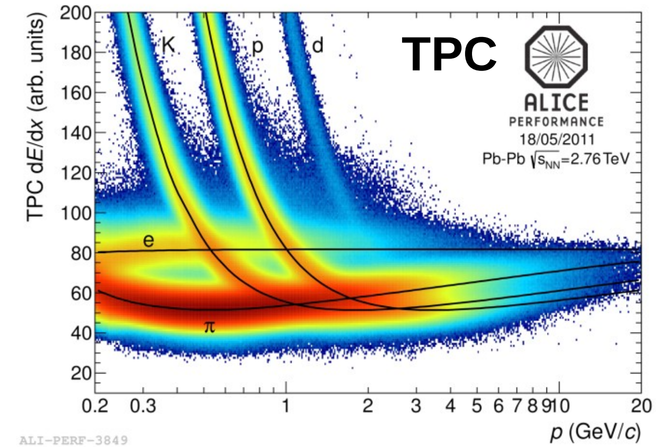
Particle identification

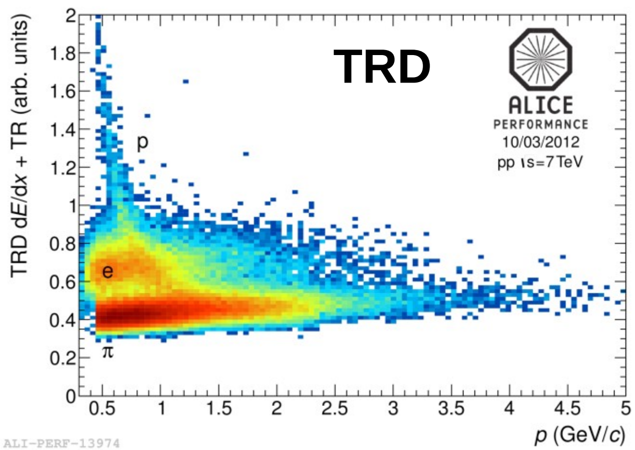
- Particle identification (PID) is one of the most important steps in many physics analyses
- Crucial for Quark-Gluon Plasma measurements
- PID is one of the strongest advantages of ALICE:
  - practically all knows techniques used (dE/dx energy loss, time-of-flight, Cherenkov radiation for hadrons and transition radiation for electrons)
  - possibility to identify (anti-)nuclei
  - very good separation of pions, kaons, protons, electrons over a wide momentum range
  - separation of signals of charged hadrons and electrons for very low momenta (down to 0.1 GeV/c)

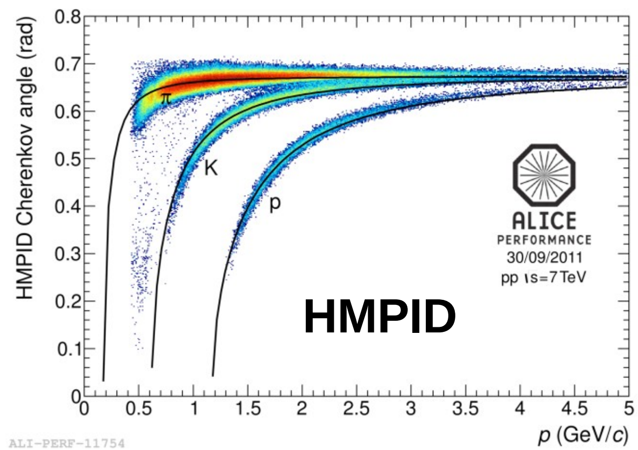
Particle identification

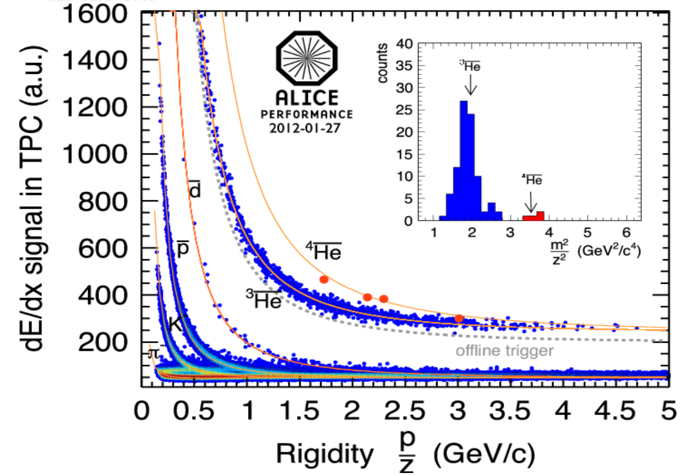


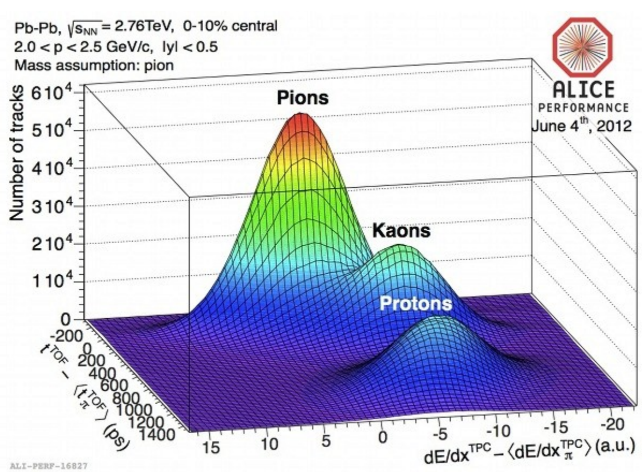






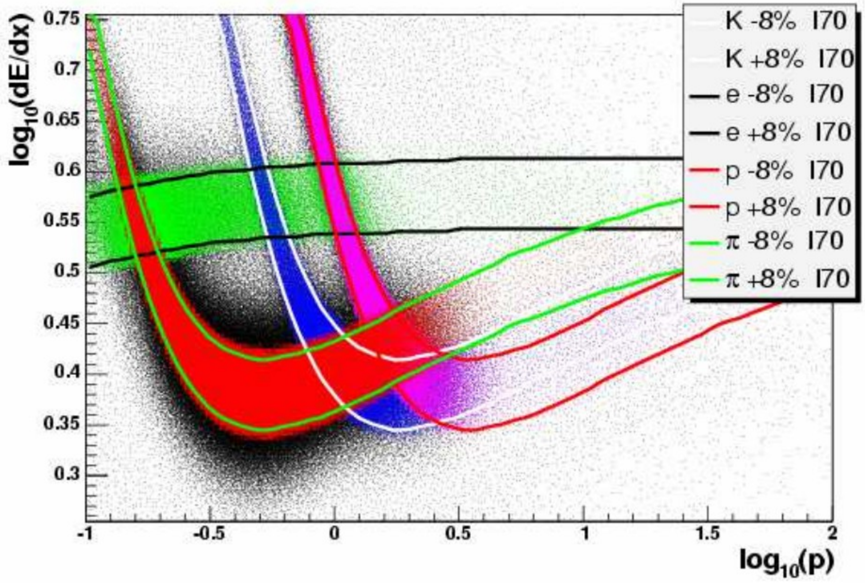






Traditional vs ML PID

- **Traditional PID:**
  - a typical analyzer selects particles "manually" by cutting on certain quantities, like the number of standard deviations of a signal from the expected value (nσ)
  - most limitations come in the regions where signals from different particle species cross
  - "cut" optimization is a time-consuming task



https://arxiv.org/pdf/nucl-ex/0505026.pdf

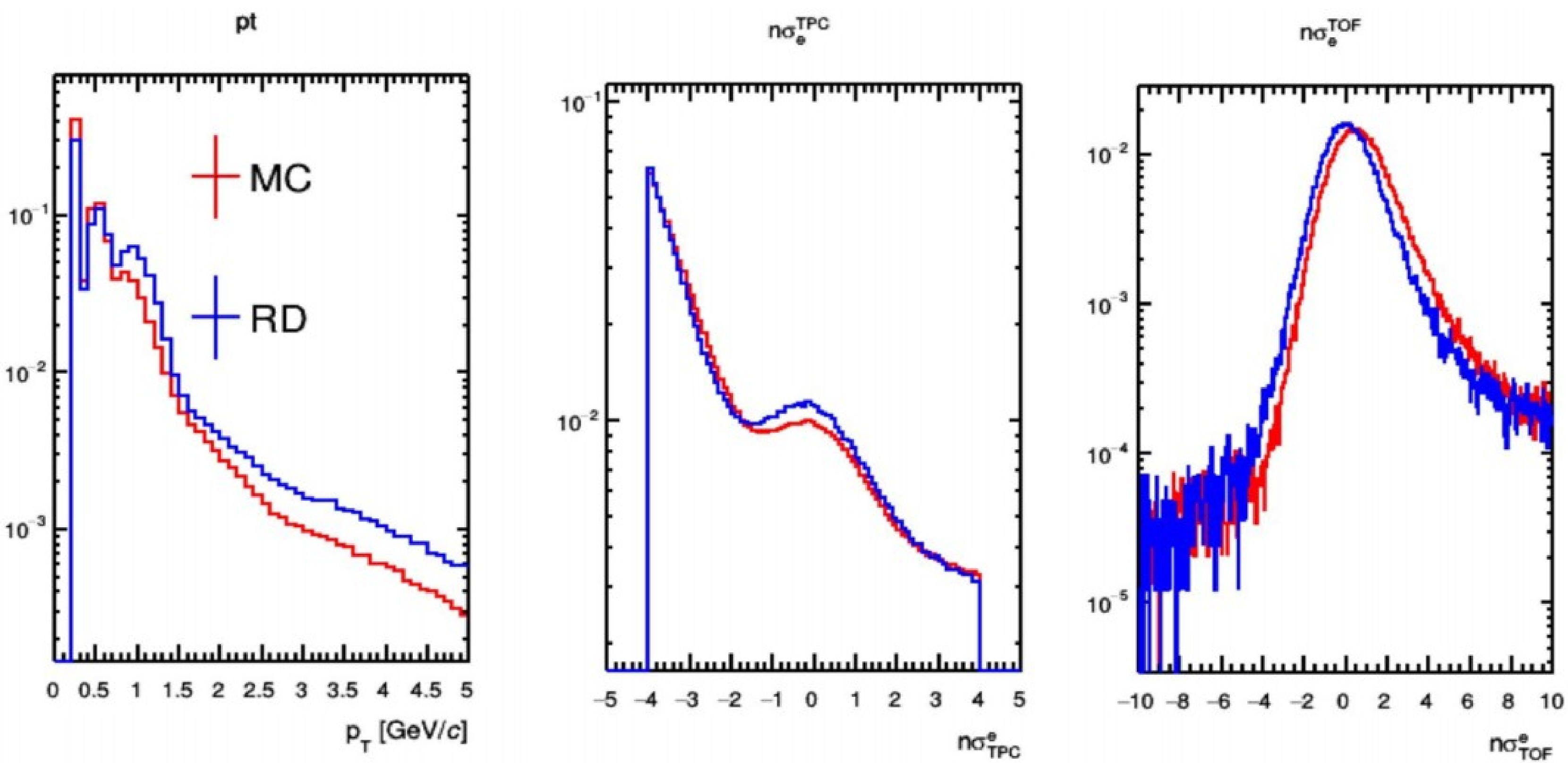
- **Machine learning PID:**
  - perfect task for machine learning
  - can learn non-trivial relations between different track parameters and PID
  - no "trial and error" approach

Proposed solution for PID

- **Build a ML classifier that can outperform traditional PID**
- **Train and validate the classifier on Monte Carlo and real data**
- **Create a simple interface for users (ALICE physicists):**
  - first attempts in 2019 (Random Forest) for LHC Run 2 (AliRoot)
    → proof-of-concept work
  - new, much more advanced, project for LHC Run 3 (O^2)
    → still in research phase
- **Limitations:**
  - Quality of the classifier will depend on the MC sample (need to handle discrepancies between data and MC)
    → no MC reweighting done
  - No easy way to calculate systematic uncertainties from the procedure
  - The classifier is a "black box" - no easy way to tell what's going on inside

Differences MC vs real data

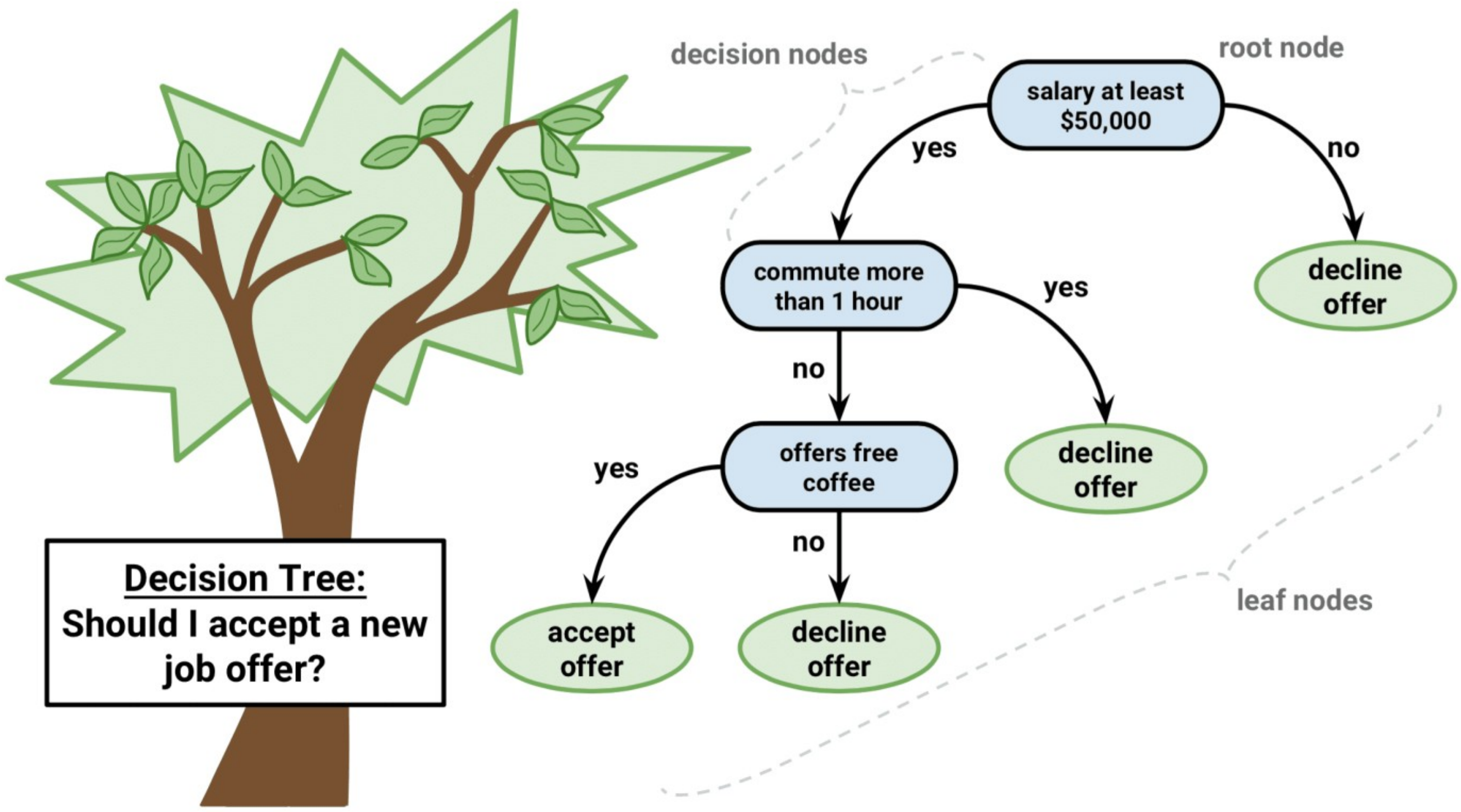
- The MC distributions don't usually reflect real data shapes
- This could potentially have an effect on the quality of identification



LHC Run 2

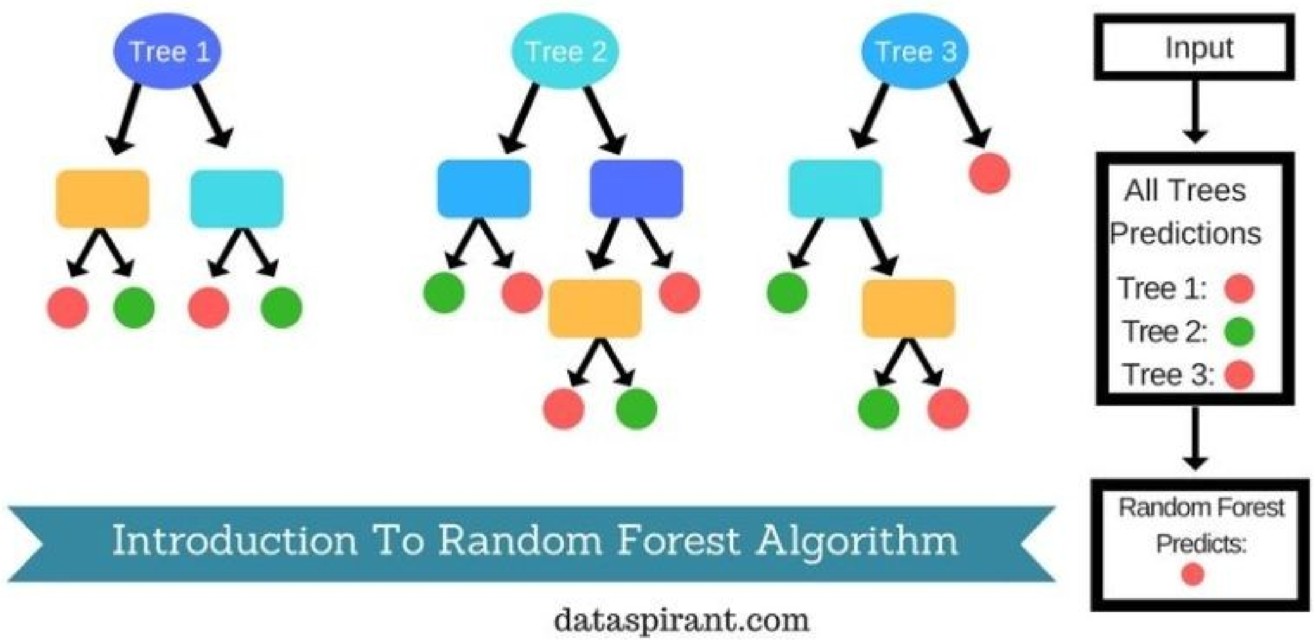
Decision tree

- A decision tree is a tree where each node represents a feature (attribute), each link (branch) represents a decision (rule) and each leaf represents an outcome (categorical or continues value)
- Decision tree learning uses a decision tree to go from observations about an item (attributes) to conclusions about the item's target value (leaves)



Random Forest

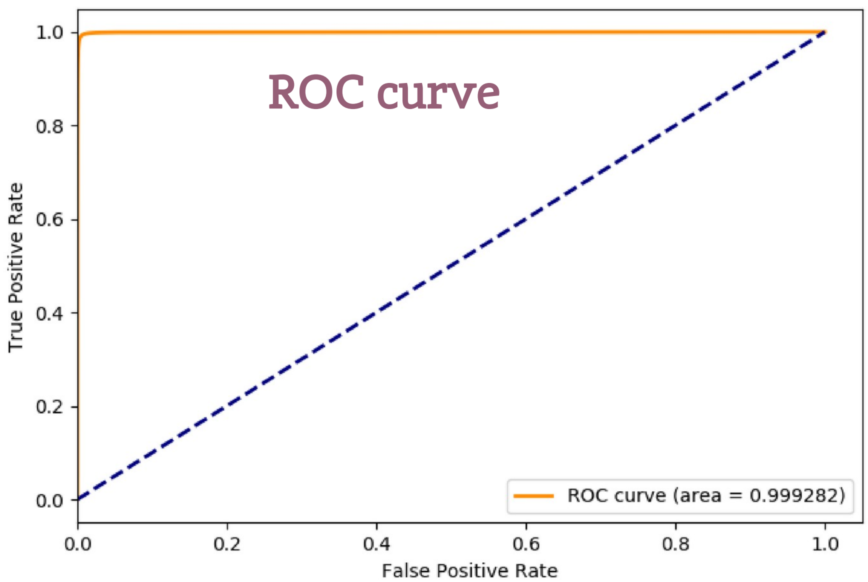
- A collection of decision trees ("forest") where each tree votes for a final decision
- Each tree is trained on a subset of randomly selected training data
- The final result is (in most cases) the one with majority of votes
- ... in addition, adaptive boosting was used

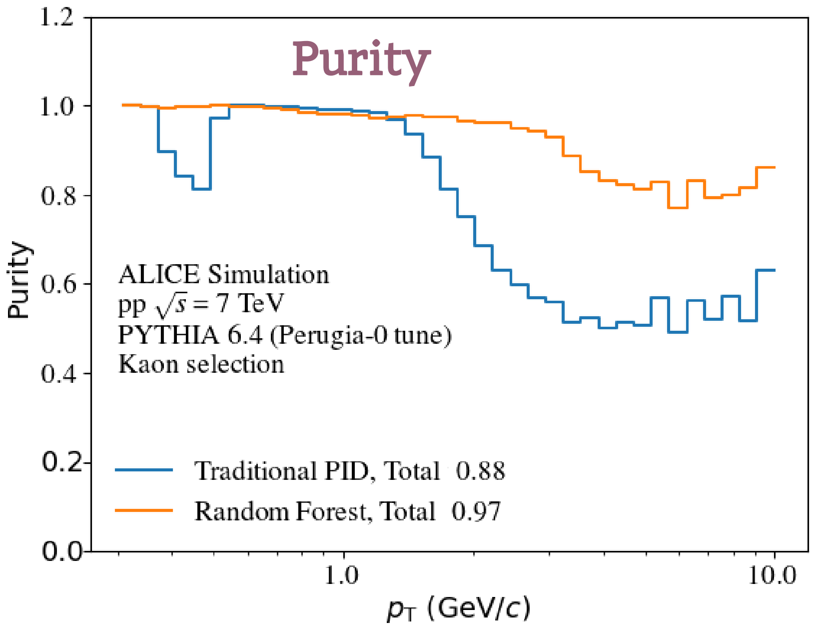


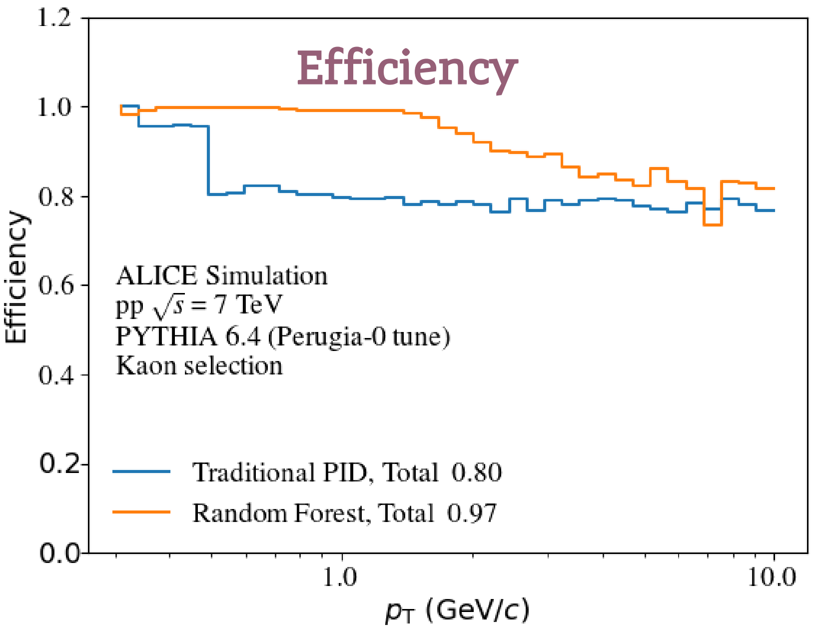
Preliminary results

Results

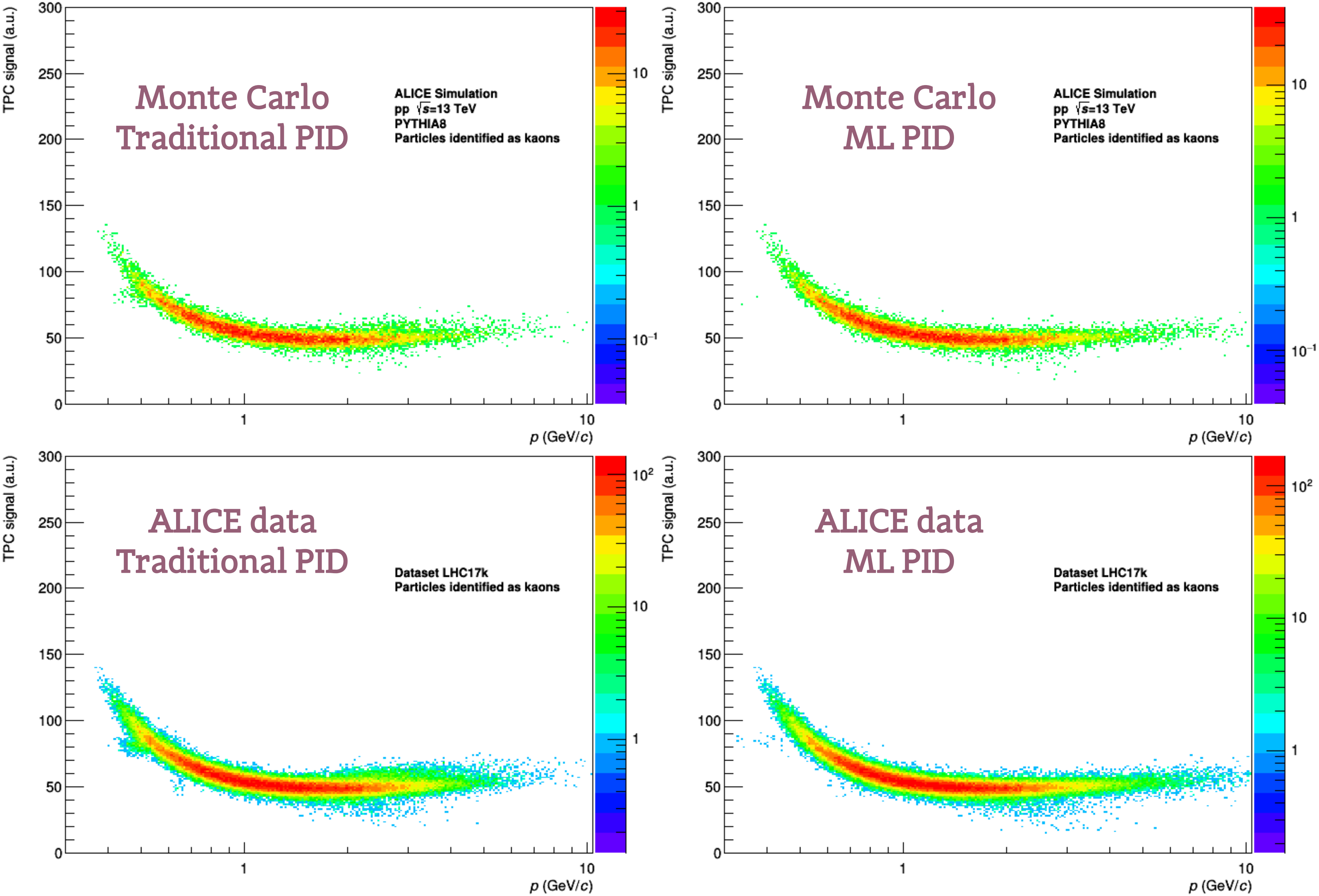
- **Test data sample:**
  - pp @ 7 TeV, Pythia 6 Perugia-0
- **Traditional PID:**
  - $n^2_{\sigma,TPC} < 2$, for $p_T \leq 0.5$ GeV/c
  - $\sqrt{n^2_{\sigma,TPC} + n^2_{\sigma,TOF}} < 2$, for $p_T > 0.5$ GeV/c
- **Machine Learning PID:**
  - Random Forest classifier



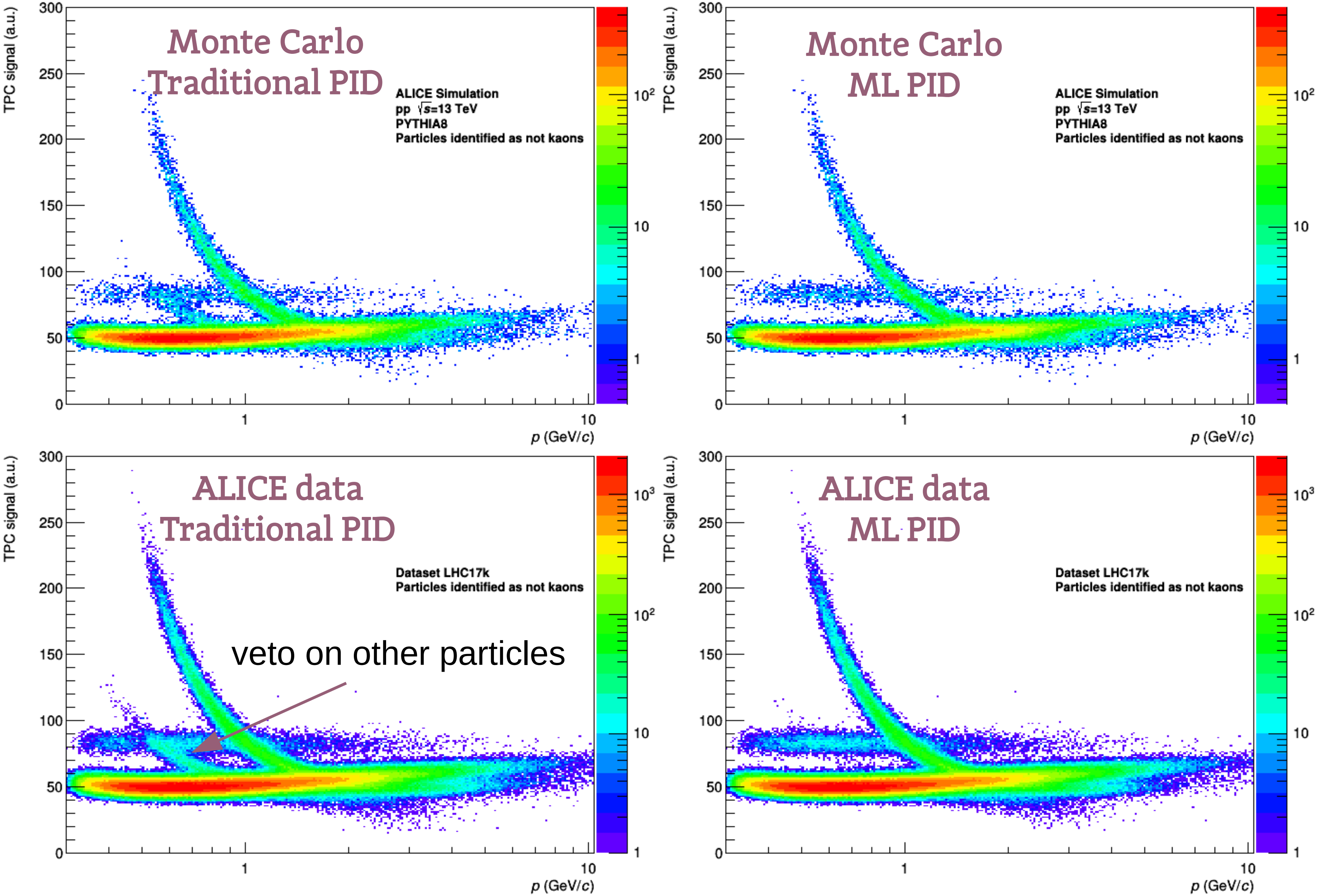




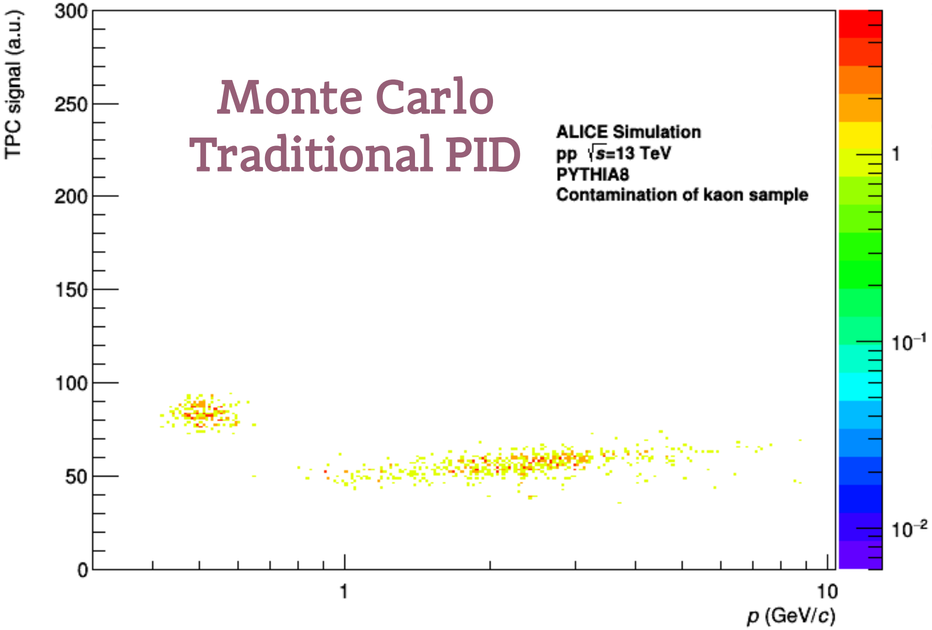
TPC accepted kaons

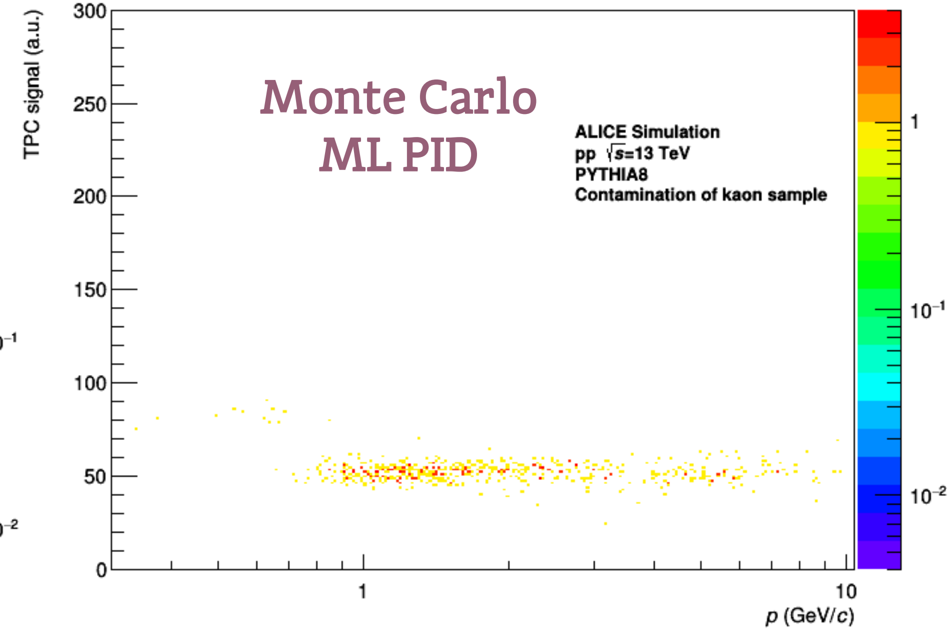


TPC rejected (not kaons)



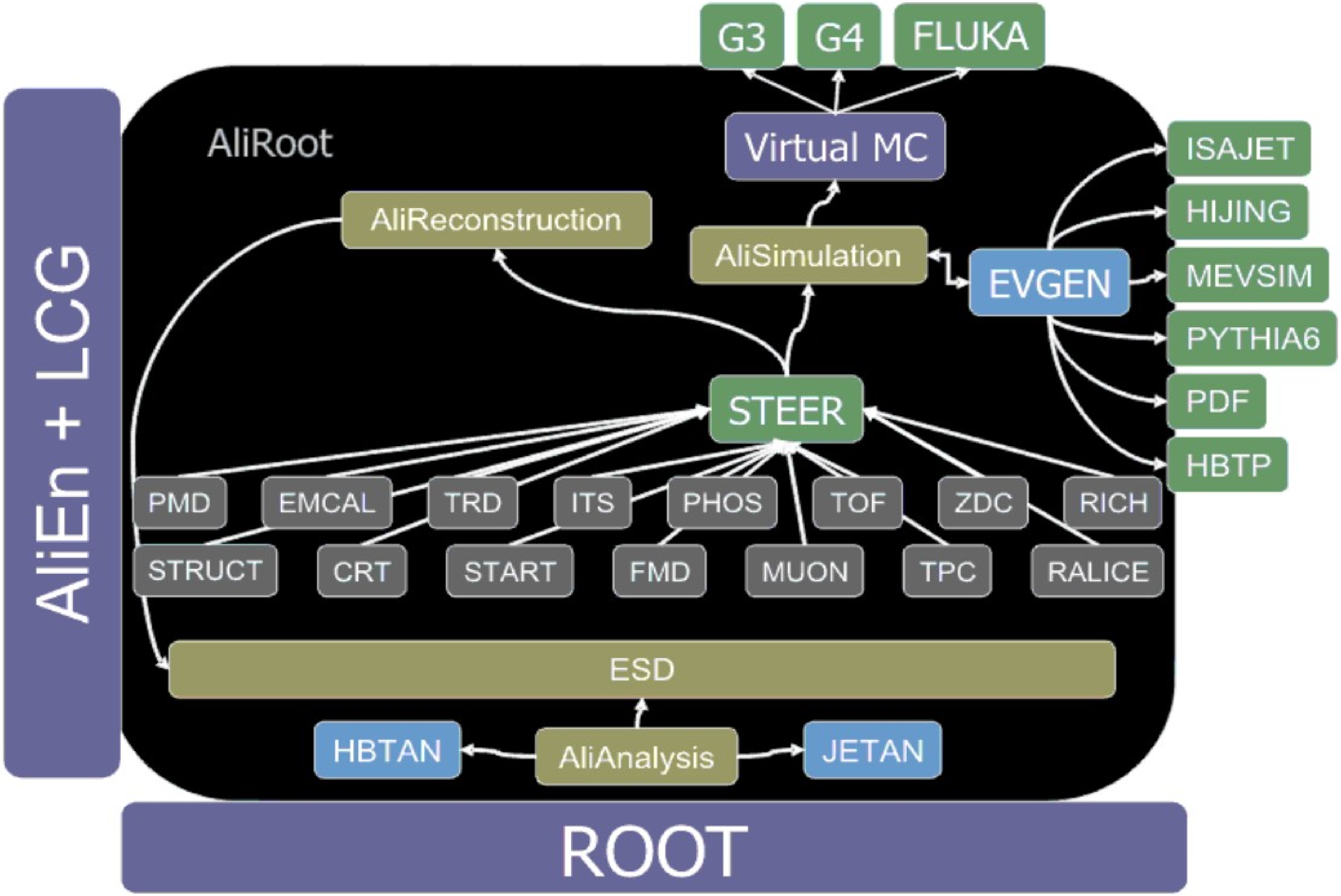
TPC contamination in kaon sample



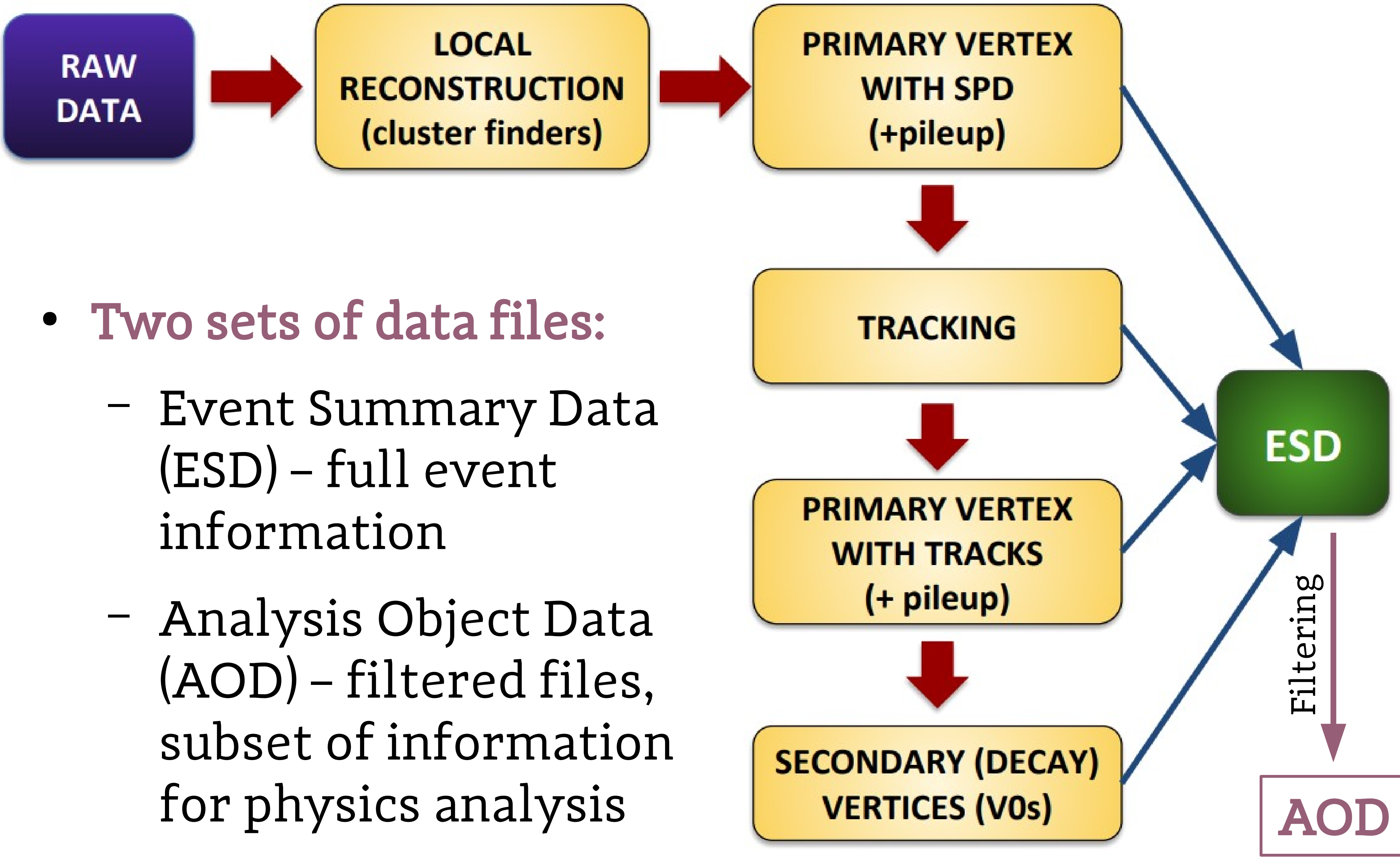


Implementation

ALICE offline framework



ALICE offline framework



- Two sets of data files:
  - Event Summary Data (ESD) – full event information
  - Analysis Object Data (AOD) – filtered files, subset of information for physics analysis

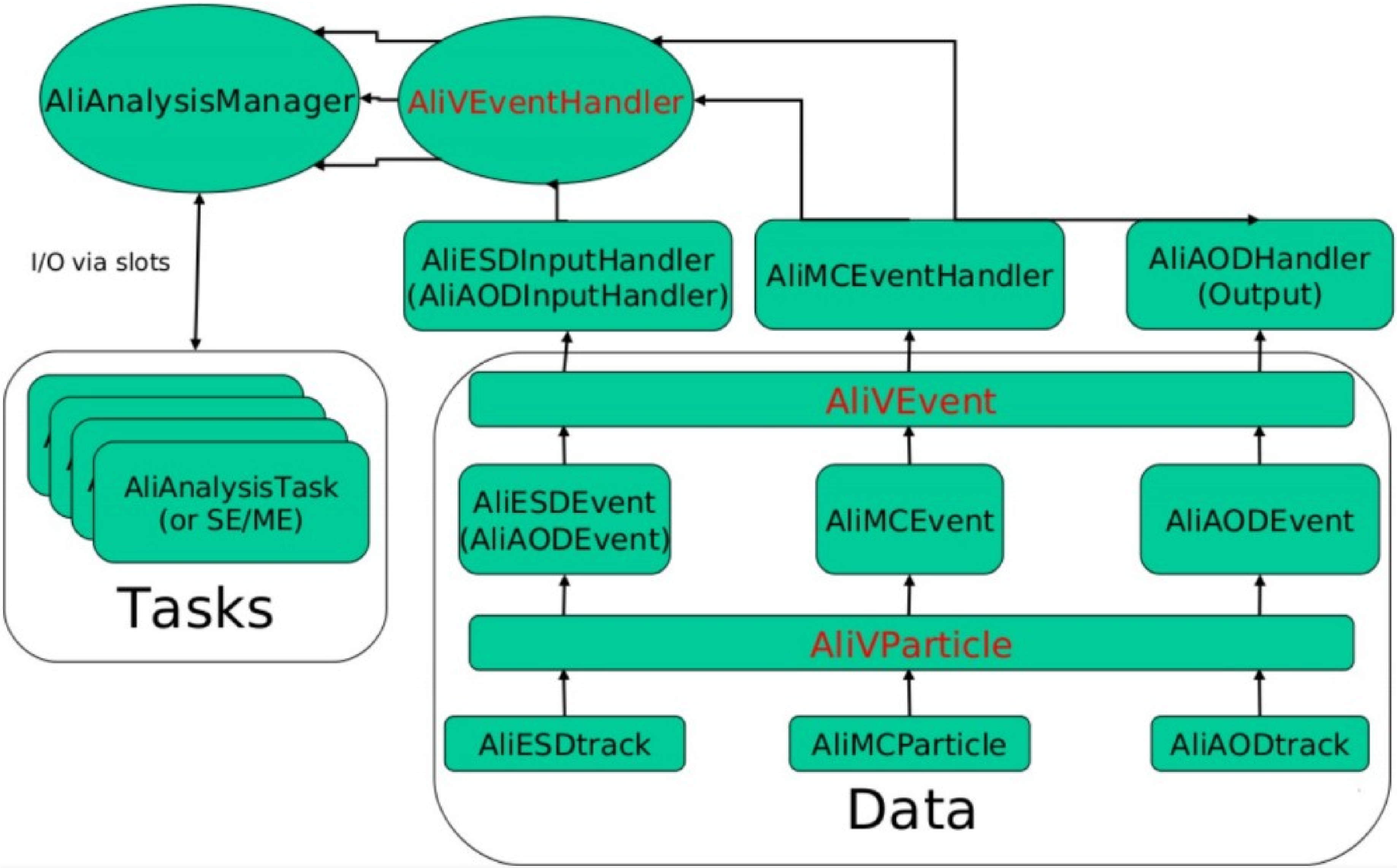
User Tasks

- Analysis is performed in an automatized way by the framework
- Users write their analysis tasks, which are specific C++ classes in AliRoot
- Framework provides iterations over files and events

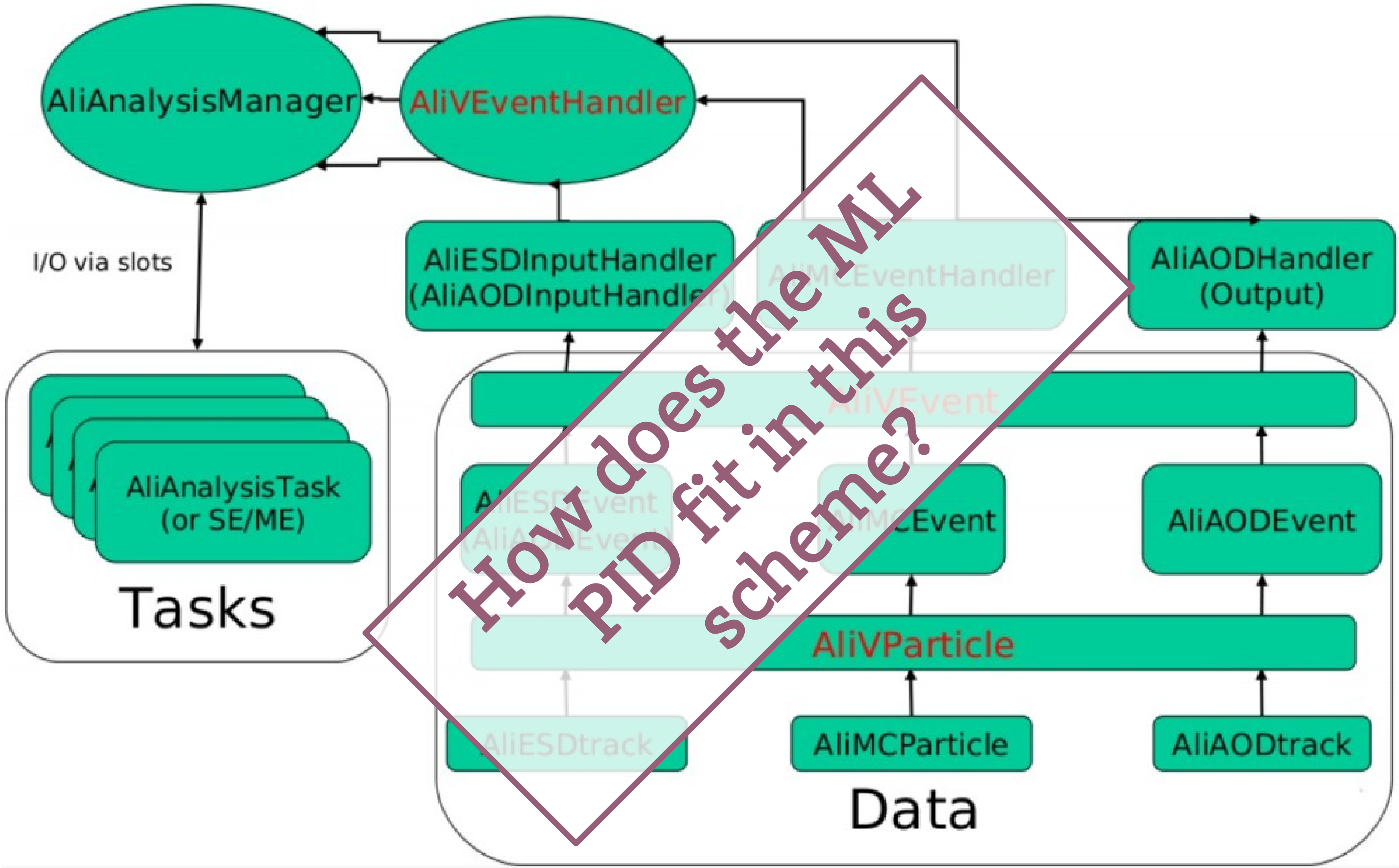
- "Constructor“* — called once on local PC
- UserCreateOutputObjects()
- UserExec() — for each event
- Terminate()

*Called in the macro

AliRoot analysis scheme



AliRoot analysis scheme

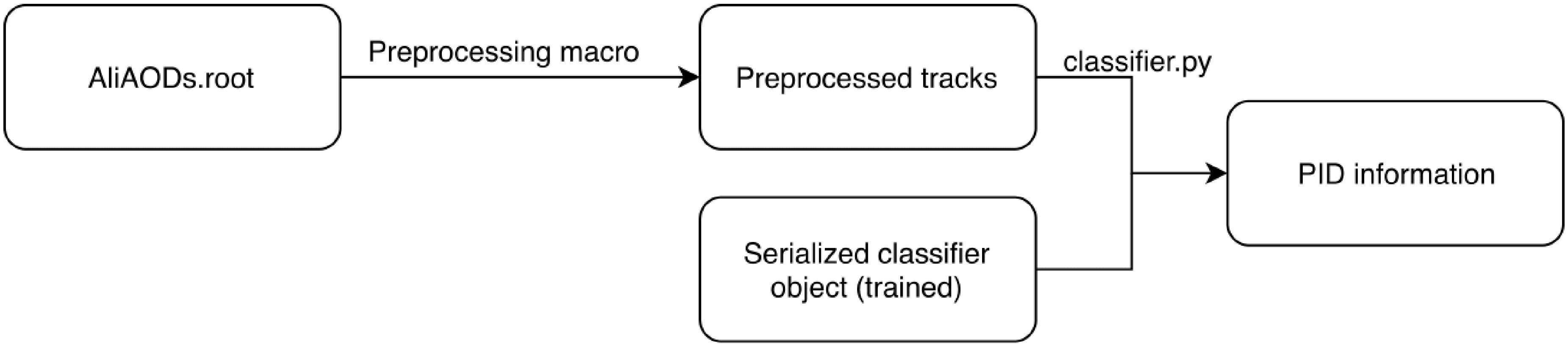


Implementation attemps

- **Training part**
  - Not covered in this talk, done externally to ALICE software
  - Proposed solution: to be done in a centralized way → not implemented finally in AliRoot
- **Classification part**
  - Classifier (in Python) prepared by an IT student
  - Implementation work in AliRoot by a physics student
  - Different attempts tested based on framework limitations
  - Demo/beta version prepared

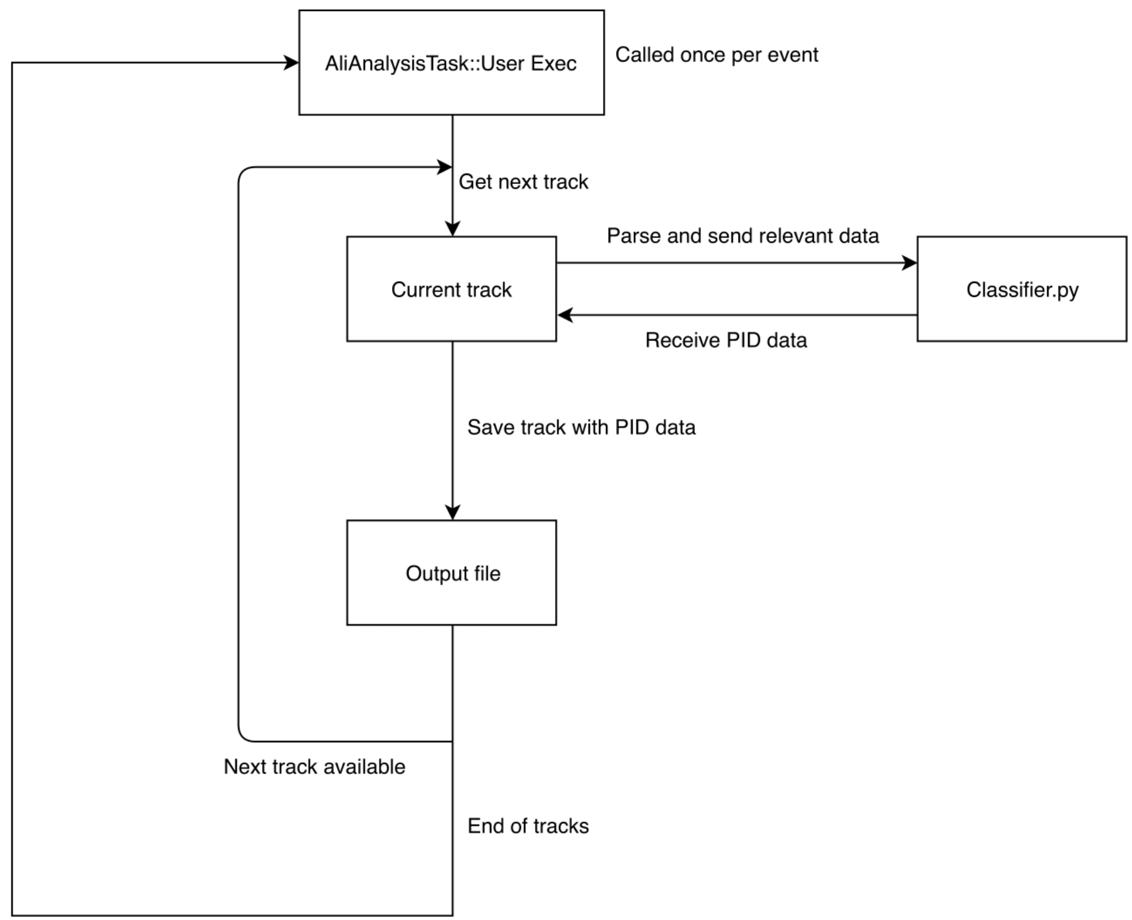
Classification – general idea

- Take tracks from AOD files and the trained model (classifier.py) in Python
- Propagate AOD tracks through the model to get the ML information for each track
- The ML PID information consists of predicted probabilities for PDG codes (pion, kaon, proton, electron, muon)
- Present the information to the user
  - via specific objects accessible in AliRoot



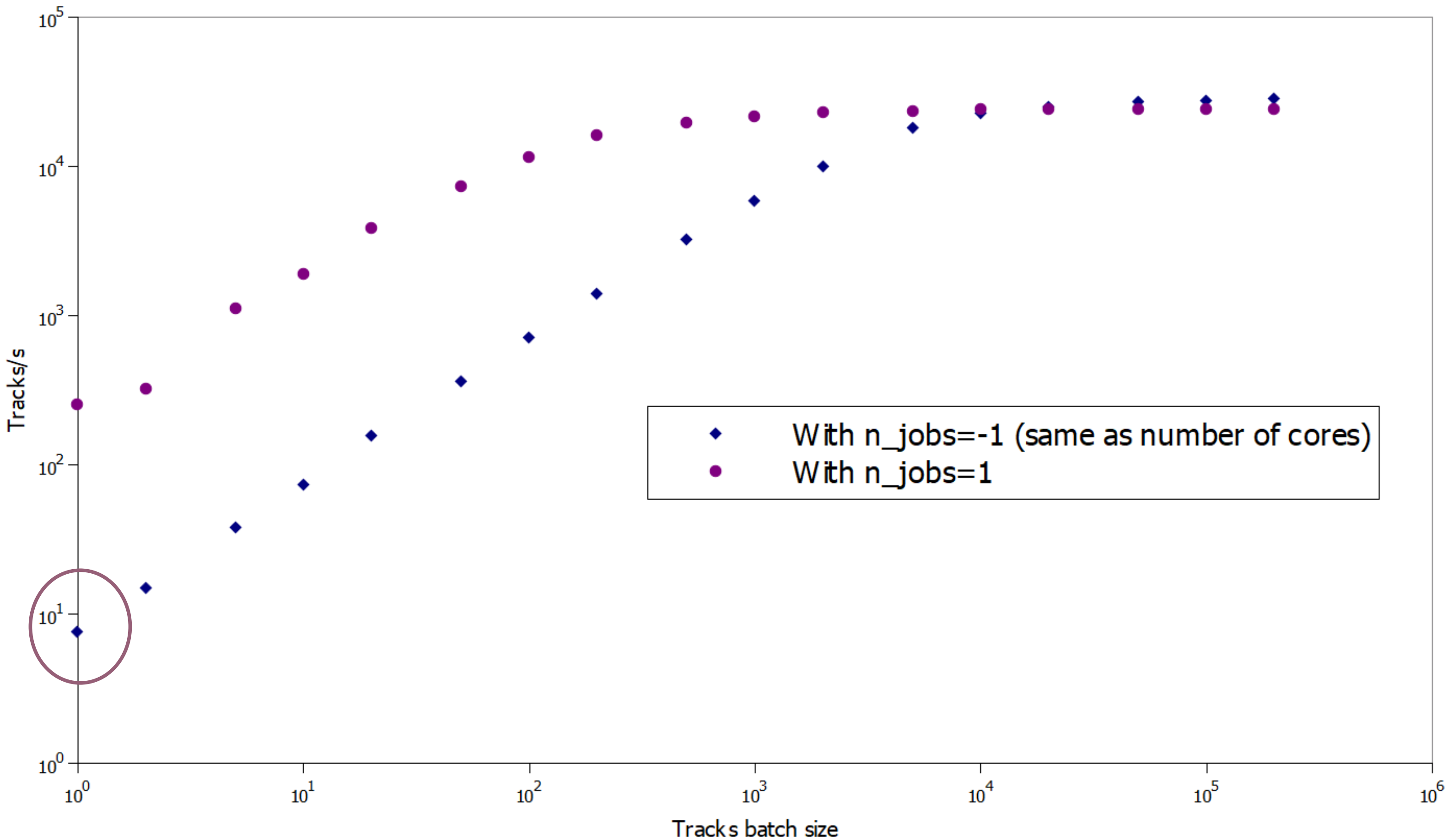
First attempt

- Track-by-track implementation
- Framework to iterate over events, loop over tracks in `UserExec()`
- Classifier listens in the background
- Stripped files sent via pipe
- PID results received via another pipe
- The method is VERY SLOW



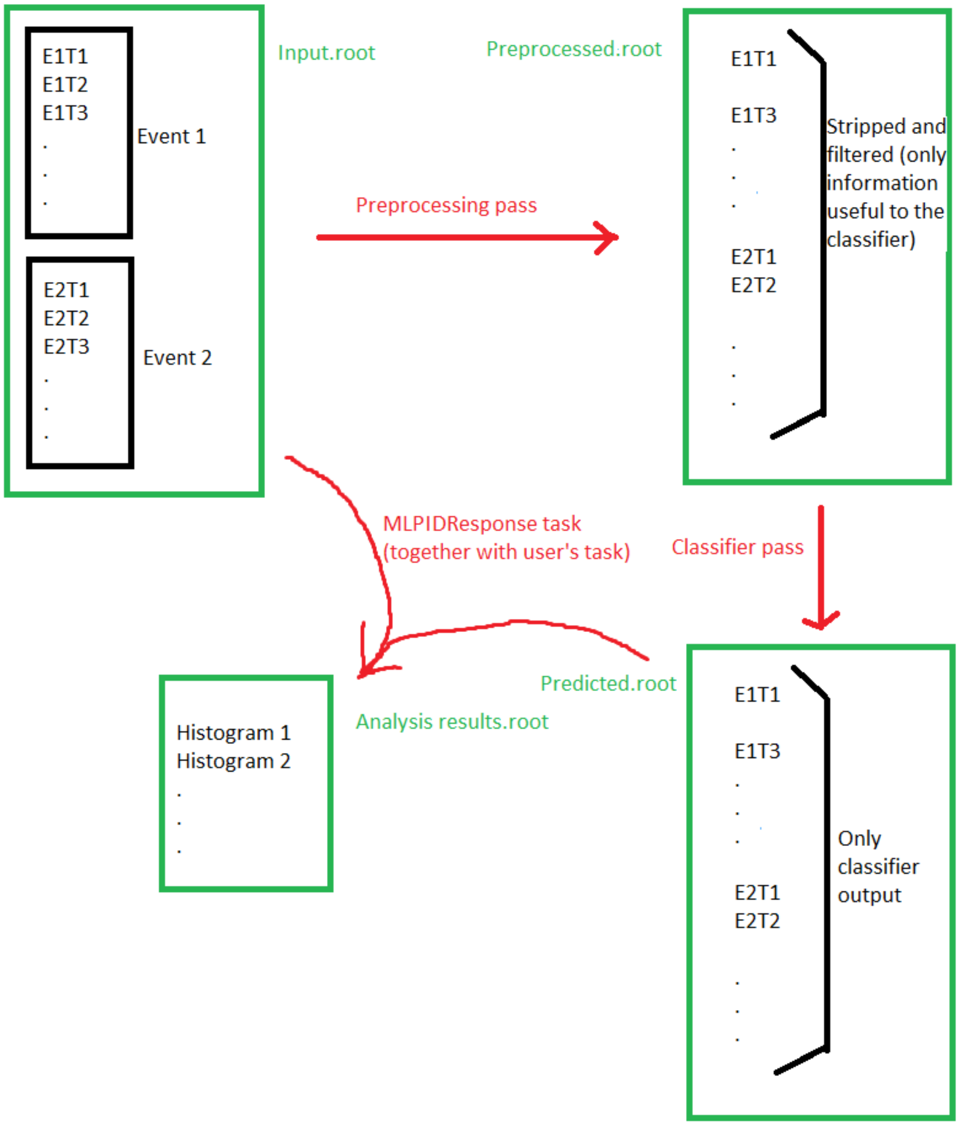
Scikit-learn benchmark

- In default track-by-track implementation, with threads, we can process <u>only ~9 tracks/s</u> (overhead from the thread creation) → no multiple threads allowed on the GRID
- Increase to more than 100 tracks/s if we do not allow threads



Second attempt

- Propagate multiple tracks through the classifier
- Two loops over events needed
  - create a temporary (stripped) file
  - propagate the temporary file through the classifier
  - produce **predicted.root** file
- In the second loop over events use a lookup table to match the two files
- Solution in AliRoot difficult (processing events twice), also slower than regular analysis



Final attempt

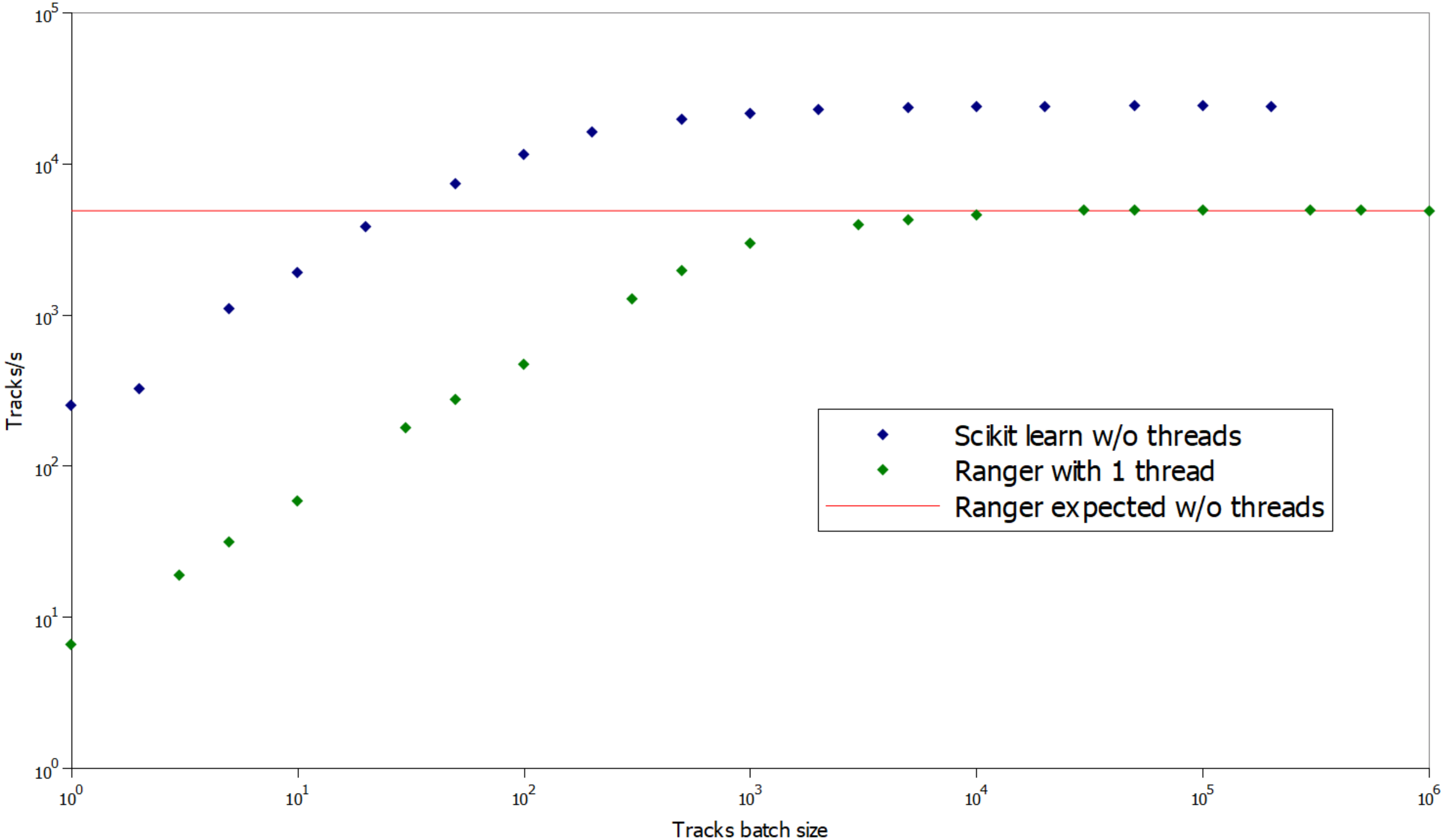
- Propagate multiple tracks through the classifier combined from <u>single events</u> (do not combine multiple events)
  - computational time of a simple p_T analysis task with ML PID (scikit-learn) and without ML PID (one 200 MB AOD file):

Real time 0:00:34 --- Without ML PID

Real time 0:01:33 --- With ML PID

  - the analysis with ML PID is **3x slower** than without ML PID
- Python interface not easily available in AliRoot, use the C++ Random Forest library (for example Ranger) instead of Python
- First tests:
  - created a "random" C++ Random Forest of the same size and depth
  - compare Ranger and scikit-learn speed tests (next slide)

Scikit-learn vs Ranger



- Ranger (C++) is <u>slower</u> than scikit-learn (Python) → Python is faster
- Ranger creates threads even when set to 1

Working demo/beta example

run macro

```
AliAnalysisTaskMLPt *myTask = new AliAnalysisTaskMLPt("MyTask");
AliAnalysisTaskMLPIDResponse *mlpidTask = new AliAnalysisTaskMLPIDResponse("MLPIDTask");

myTask->SelectCollisionCandidates(AliVEvent::kINT7);
if( !myTask )
  exit(-1);
mgr->AddTask(mlpidTask);
mgr->AddTask(myTask);

// Create containers for input/output
AliAnalysisDataContainer *cinput = mgr->GetCommonInputContainer();
AliAnalysisDataContainer *coutput2 = mgr->CreateContainer("MyTree",
        TList::Class(),AliAnalysisManager::kOutputContainer,outfilename);

//connect them to future analysis
mgr->ConnectInput(mlpidTask,0,cinput);
//mgr->ConnectOutput(mlpidTask,1,coutput2);
mgr->ConnectInput(myTask,0,cinput);
mgr->ConnectOutput(myTask,1,coutput2);

if ( !mgr->InitAnalysis() )
    return;
mgr->PrintStatus();

//start analysis
mgr->StartAnalysis("local",chain,Nevents);
```

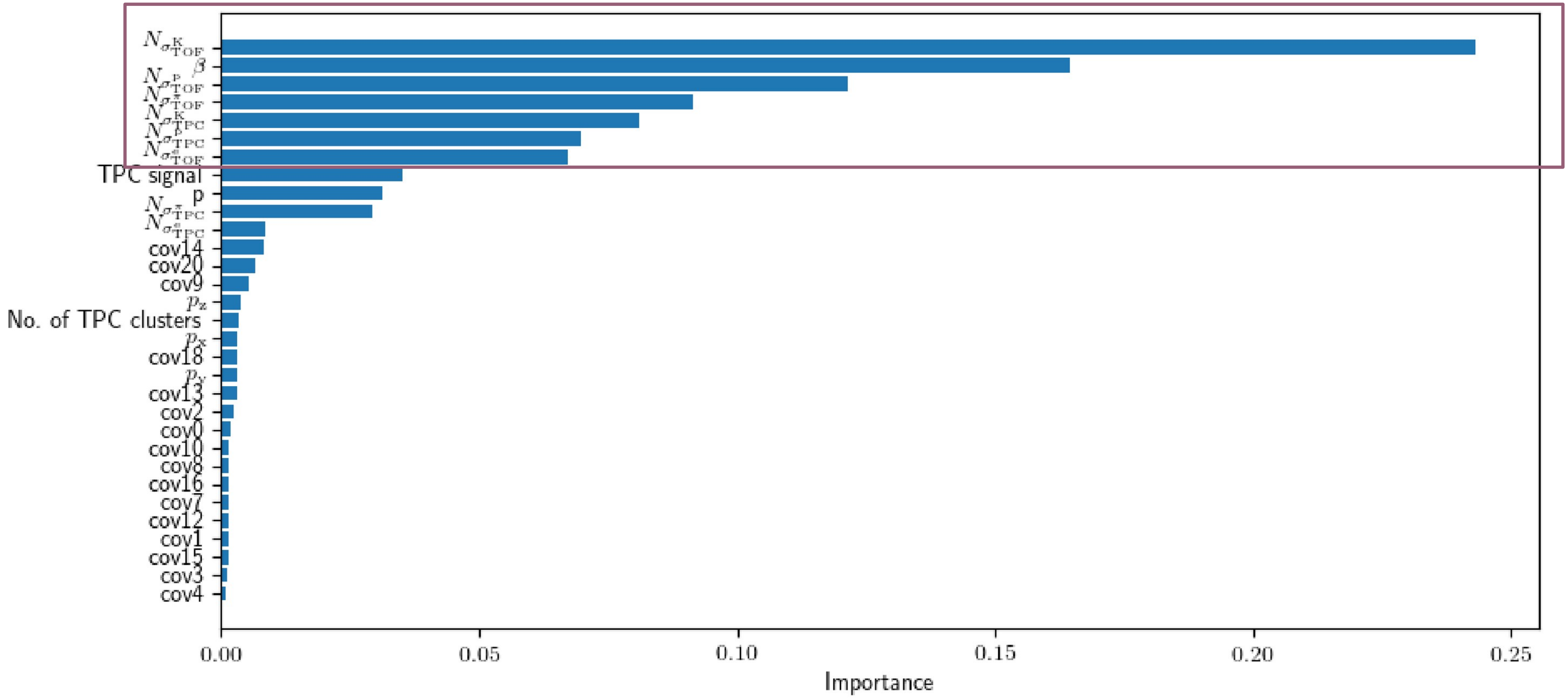
user's analysis task

```
//loop over AOD reconstructed tracks
for (Int_t iTracks = 0; iTracks < aodEvent->GetNumberOfTracks(); iTracks++) {
    //get track
    AliAODTrack *track = (AliAODTrack*)aodEvent->GetTrack(iTracks);
    if (!track)
        continue;

    UInt_t filterBit = 96;
    if(!track->TestFilterBit(filterBit))
        continue;

if (!fMLpidUtil)
  continue;

AliMLPIDResponse* resp = fMLpidUtil->getTrackPIDResponse(track->GetID());
if (!resp)
  continue;
else
  cout<<"Good PID: "<<resp->predictedPDG<<endl;


int pdg = resp->predictedPDG;
if(pdg == 211)
  ptHistPions->Fill(track->Pt());
if(pdg == 321)
  ptHistKaons->Fill(track->Pt());
if(pdg == 2212)
  ptHistProtons->Fill(track->Pt());


    //save all attributes into TTree
    //treeOutput->Fill();
}
```

- **User just needs to add a couple of lines – like for a traditional PID**
  → inclusion of the PID response task

LHC Run 3

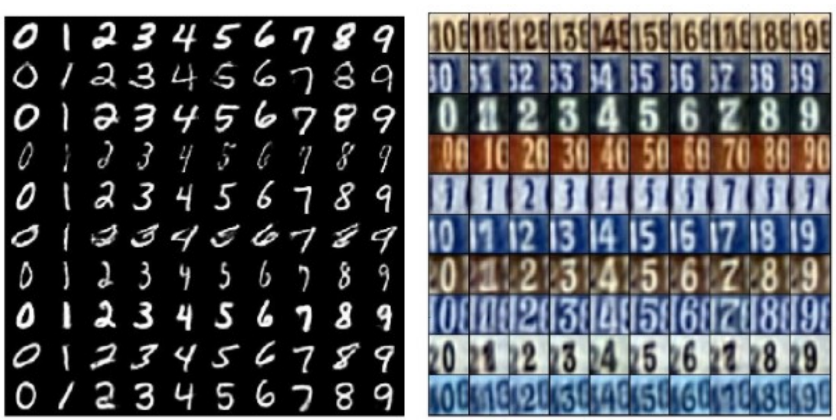
PID parameter importance



- The algorithm was trained on information from TPC and TOF parameterization (which is done before and loaded with "PID response task" in the analysis)
- ... in the LHC Run 3 we plan to use only raw signals from the detectors (TPC dE/dx, TOF time)

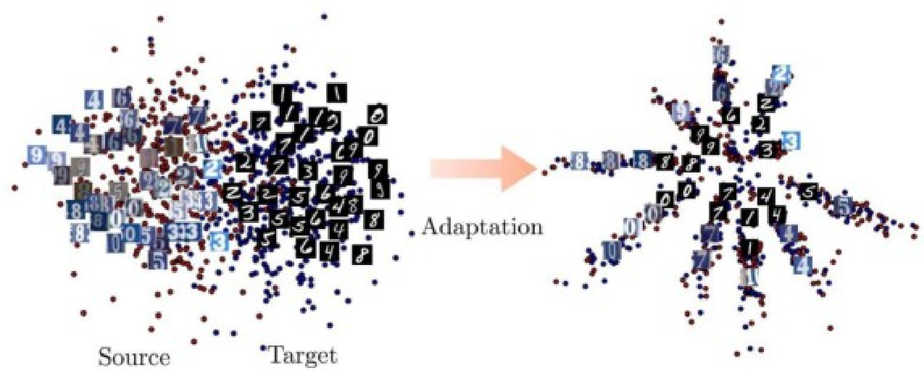
Domain adaptation

- ALICE is undergoing a major upgrade with completely new software framework O^2
- We plan to explore the Unsupervised Domain Adaptation for ML PID
  - problem of transferring the knowledge from a **labeled source domain** to **unlabeled target domain**, when both domains have different distributions of attributes (as in the case of MC and data)
- No implementation in O^2 yet, research work ongoing



(a) MNIST (b) SVHN

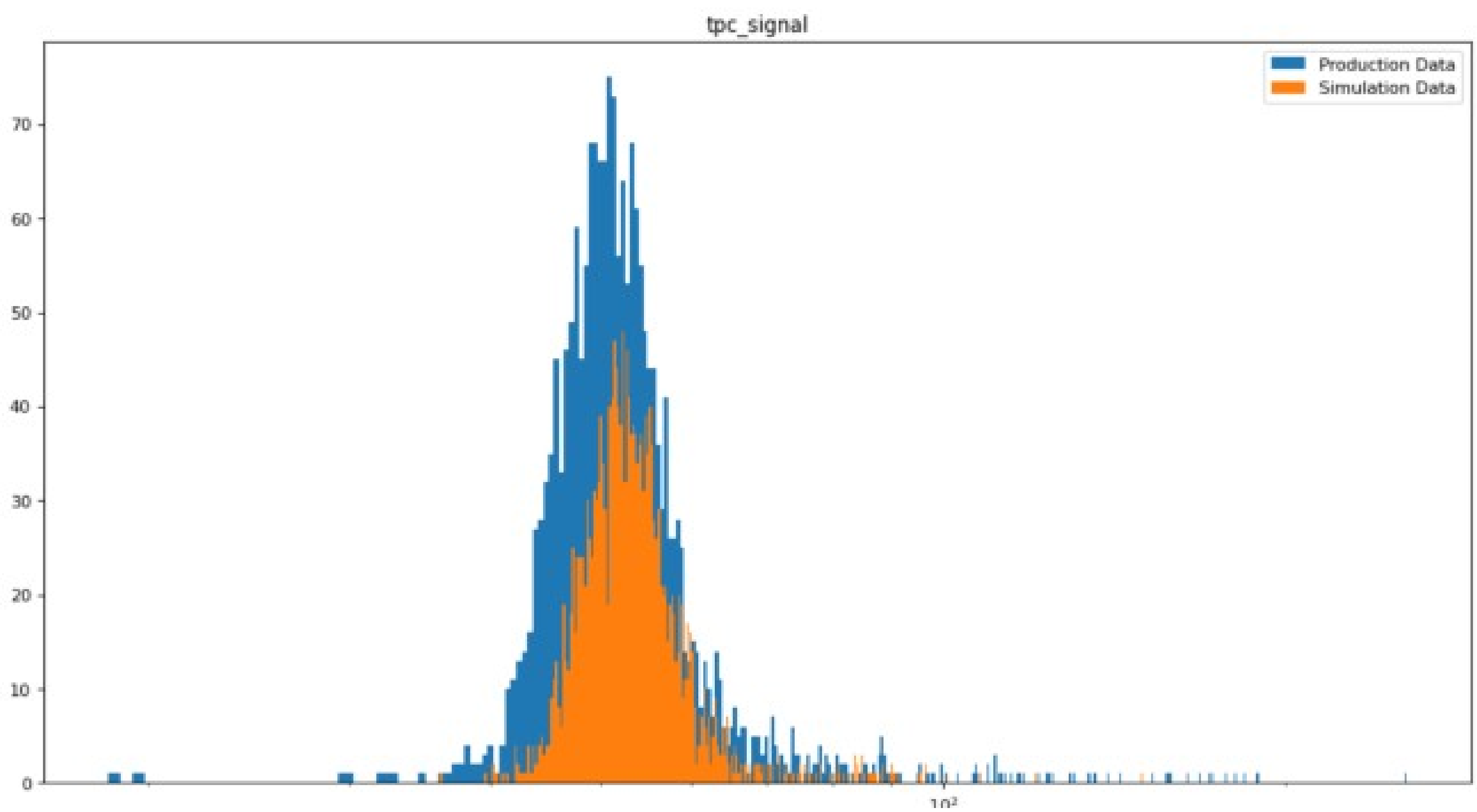
MNIST and SVHN datasets



Visualization of domain adaptation

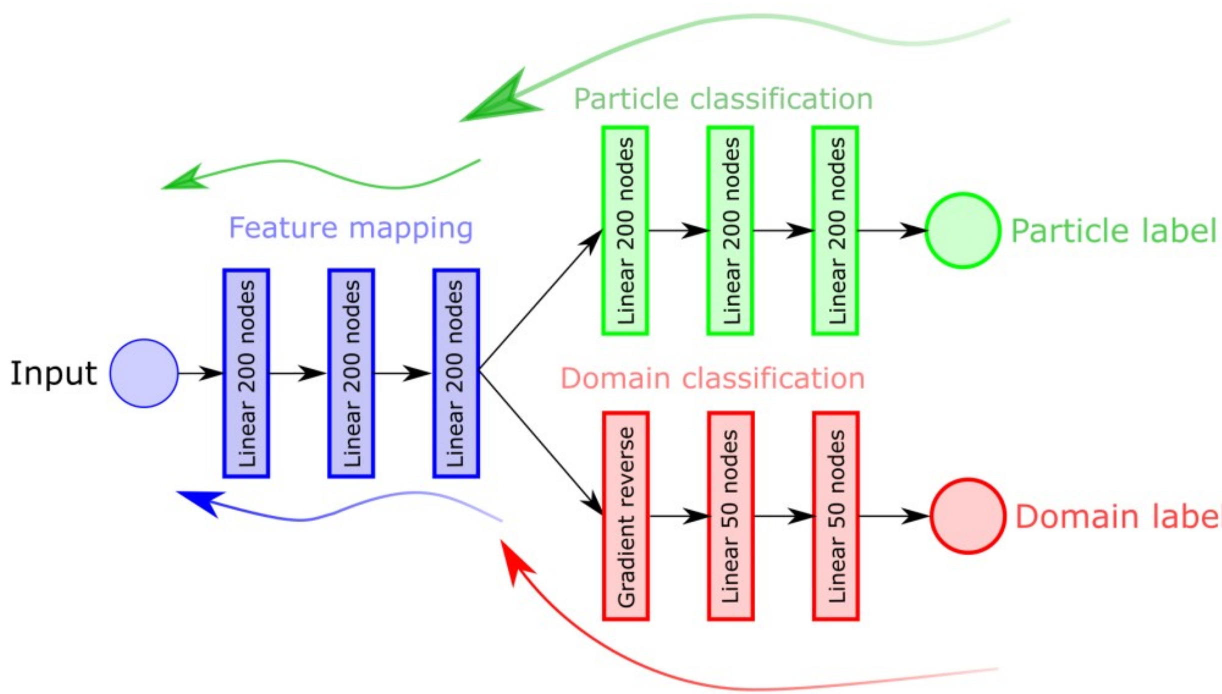
Domain adaptation

- Example domain shift between MC simulated and real data (TPC signal)

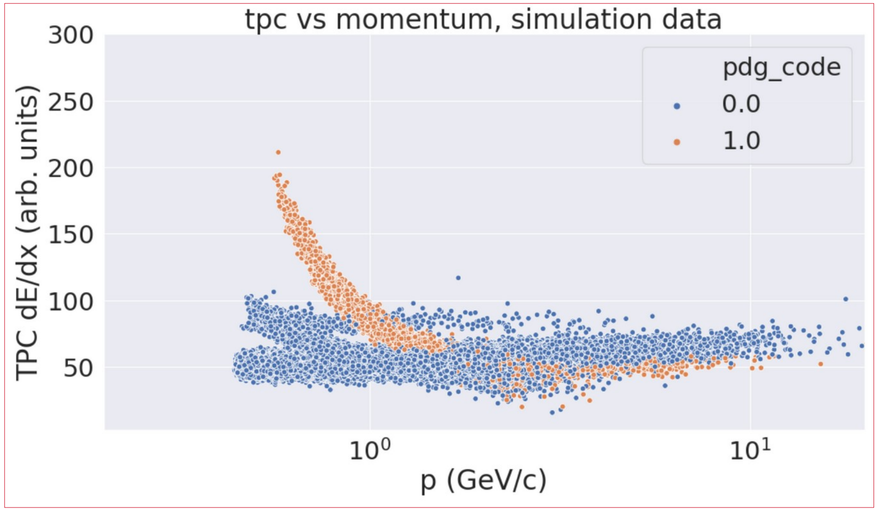


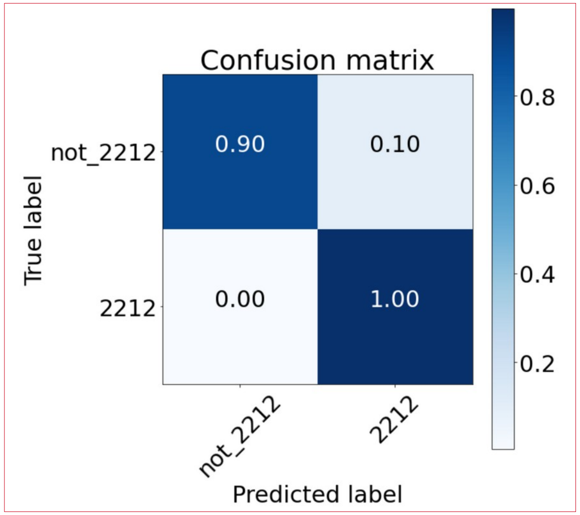
Proposed model

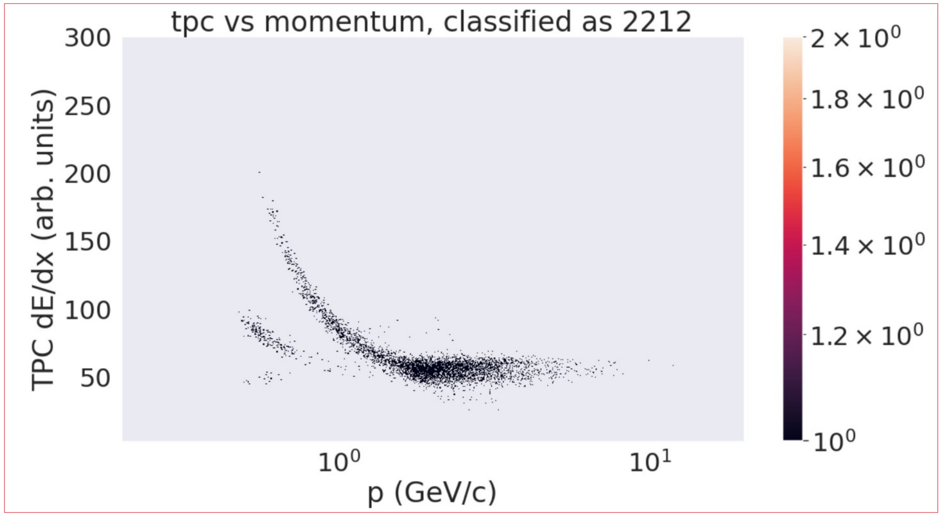
- One versus all based model based on Domain Adversarial Training of Neural Networks
- Architecture consists of three neural networks:
  - **feature mapping network**, which maps features of both data sets into common, domain invariant latent space
  - **particle classification network**, which classifies particles basing on domain invariant latent space
  - **domain discriminator network**, which classifies domain of each particle



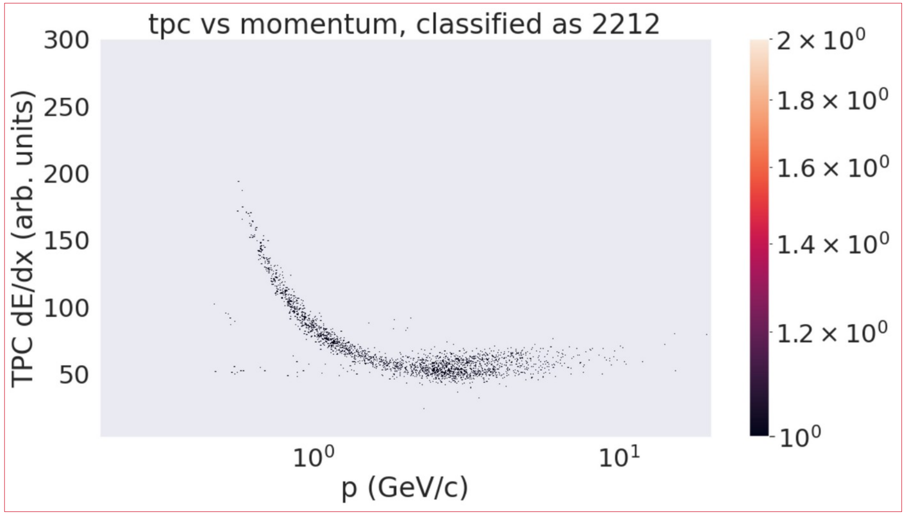
First results – proton selection







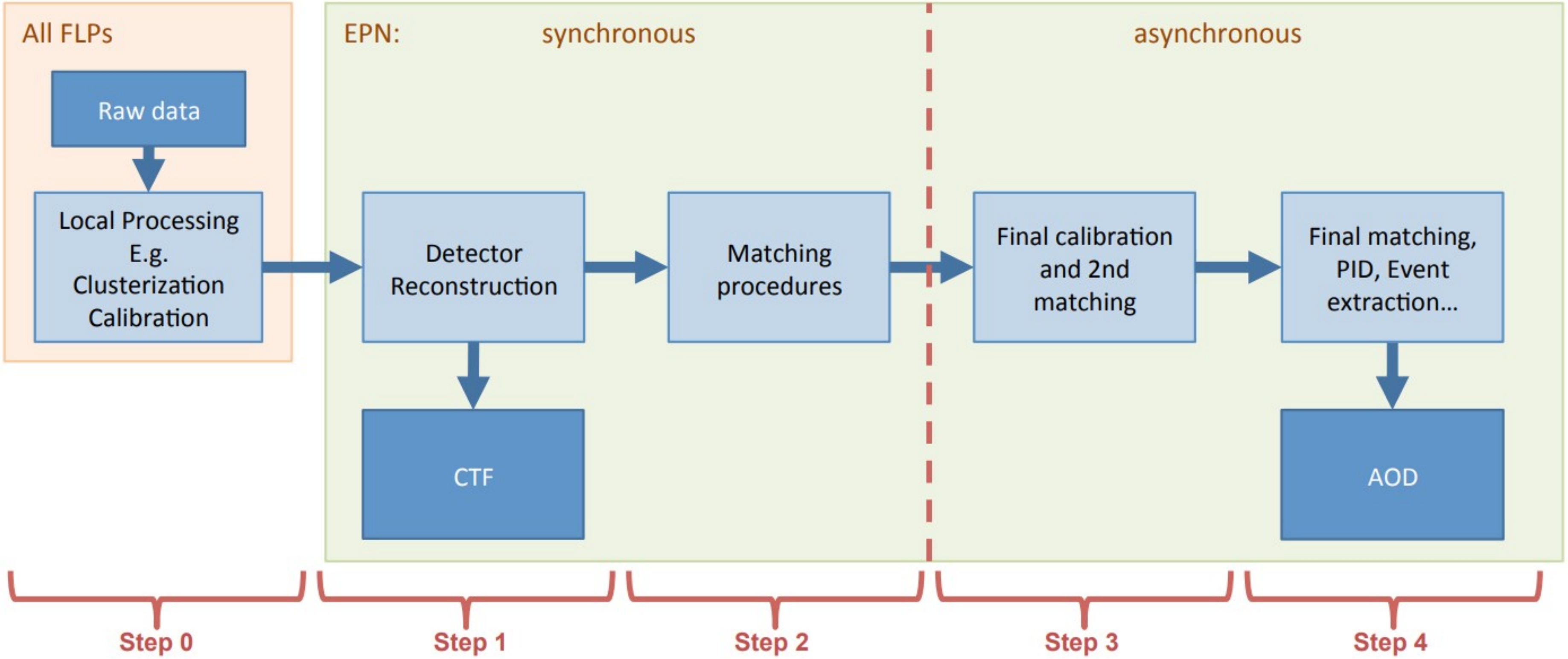
No Domain Adaptation



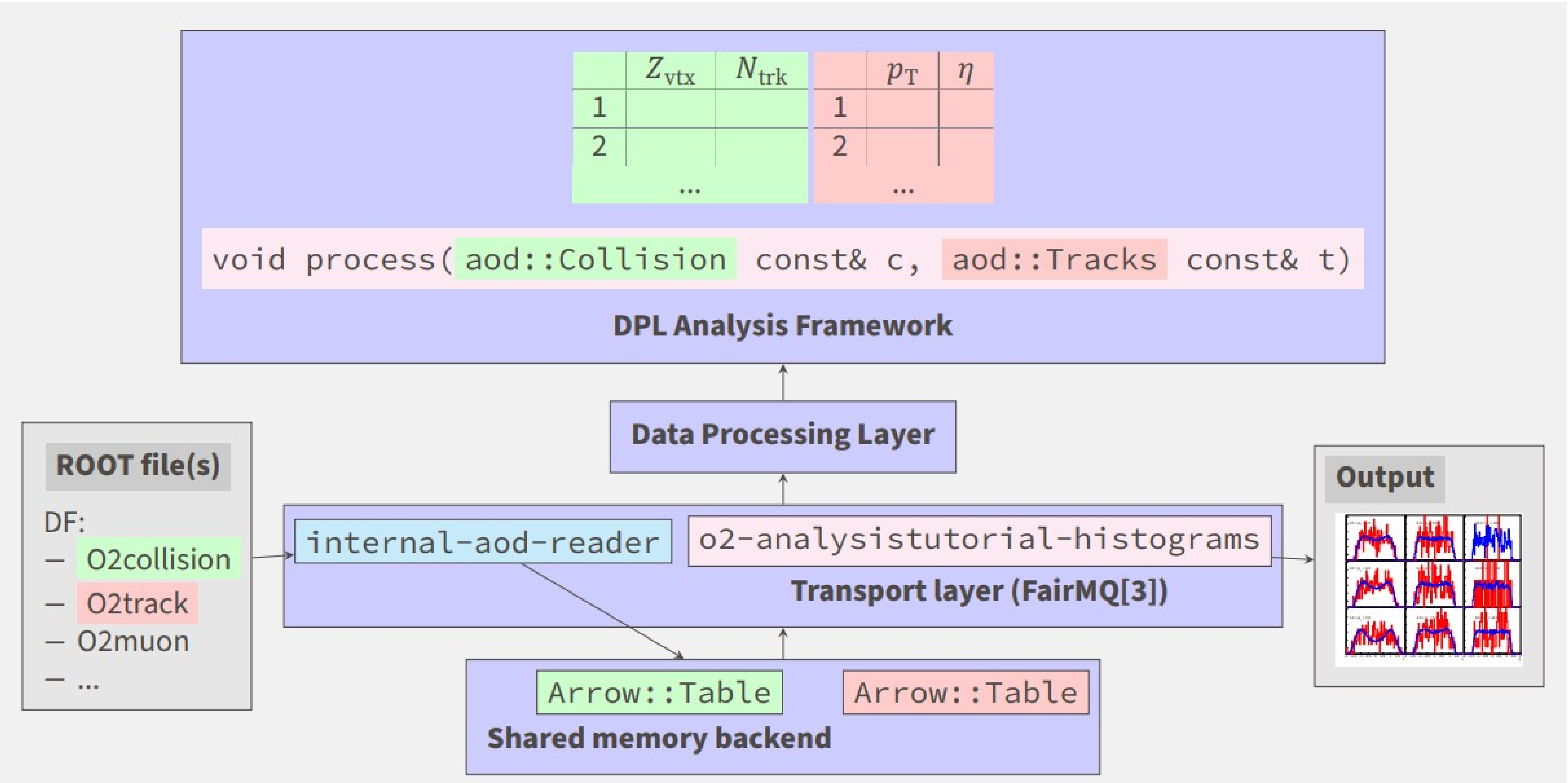
Domain Adaptation

LHC Run 3 computing (O^2)

- x100 higher data rate
- (Updated) AOD format – calculate as much as possible on-the-fly
- O2 Data Processing Layer (DPL)
  - coherent framework from data taking to analysis
- Input data - flat tables (sets of columns) stored as flat ROOT trees



LHC Run 3 computing (O^2)



Anton Alkin, vCHEP 2021
https://indico.cern.ch/event/948465/contributions/4324158/

LHC Run 3 computing (O^2)

- Example analysis task

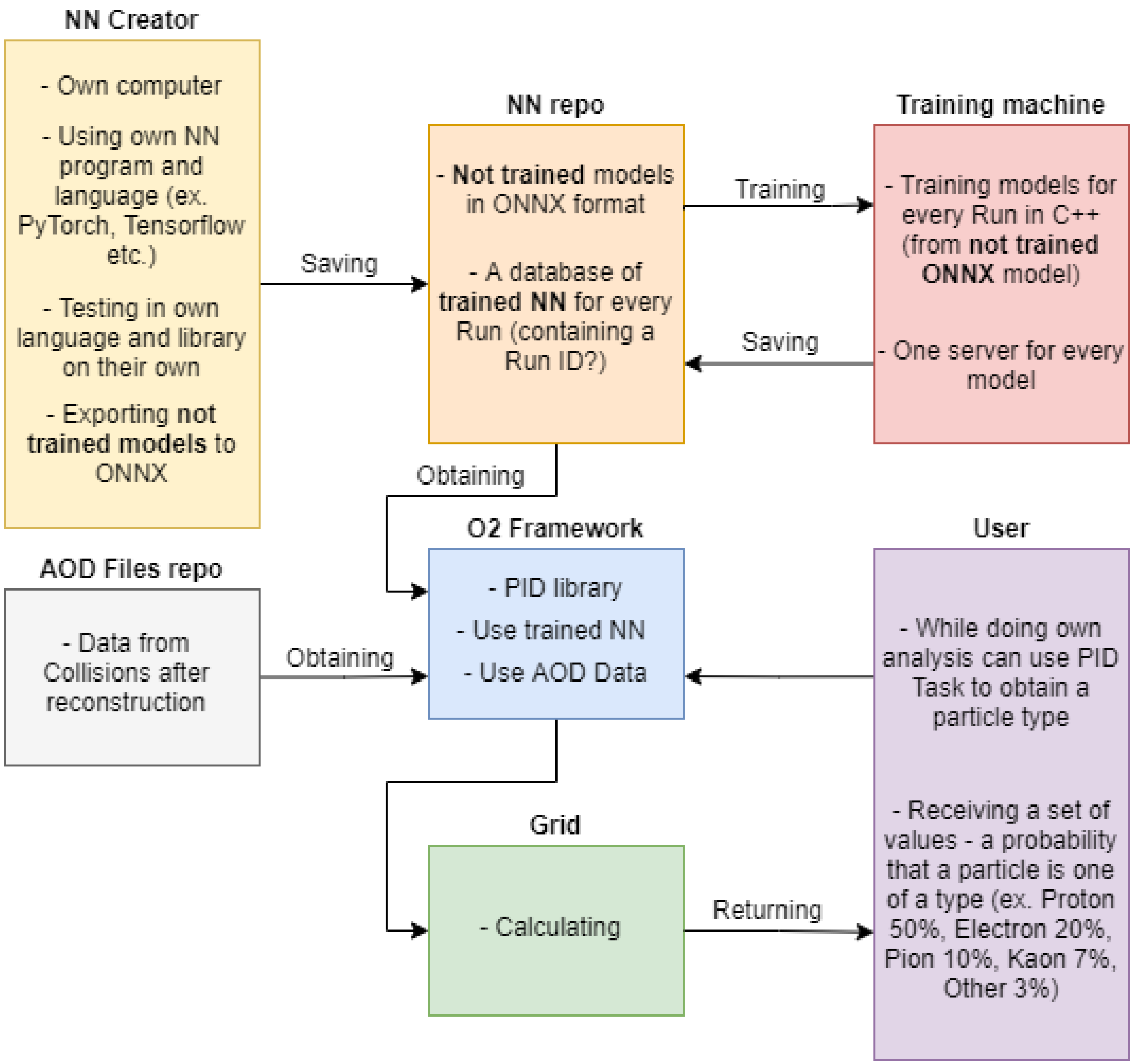
```
struct ATask {
  OutputObj<TH2F> etaphiH{TH2F("etaphi", "etaphi", 100, 0., 2. * M_PI,
102, -2.01, 2.01)};
  Configurable<float> phiCut{"phiCut", 6.29f, "A cut on phi"};
  Filter phiFilter = (track::phi < phiCut)

  void process(soa::Filtered<Tracks> const& tracks)
  {
    for (auto& track : tracks) {
      etaphiH->Fill(track.phi(), track.eta());
    }
  }
};
```

Only filtered tracks

- Our ML PID model has to fit in this scheme!

Implementation

- ONNX discussed to be used for storing trained networks
- Very preliminary scheme

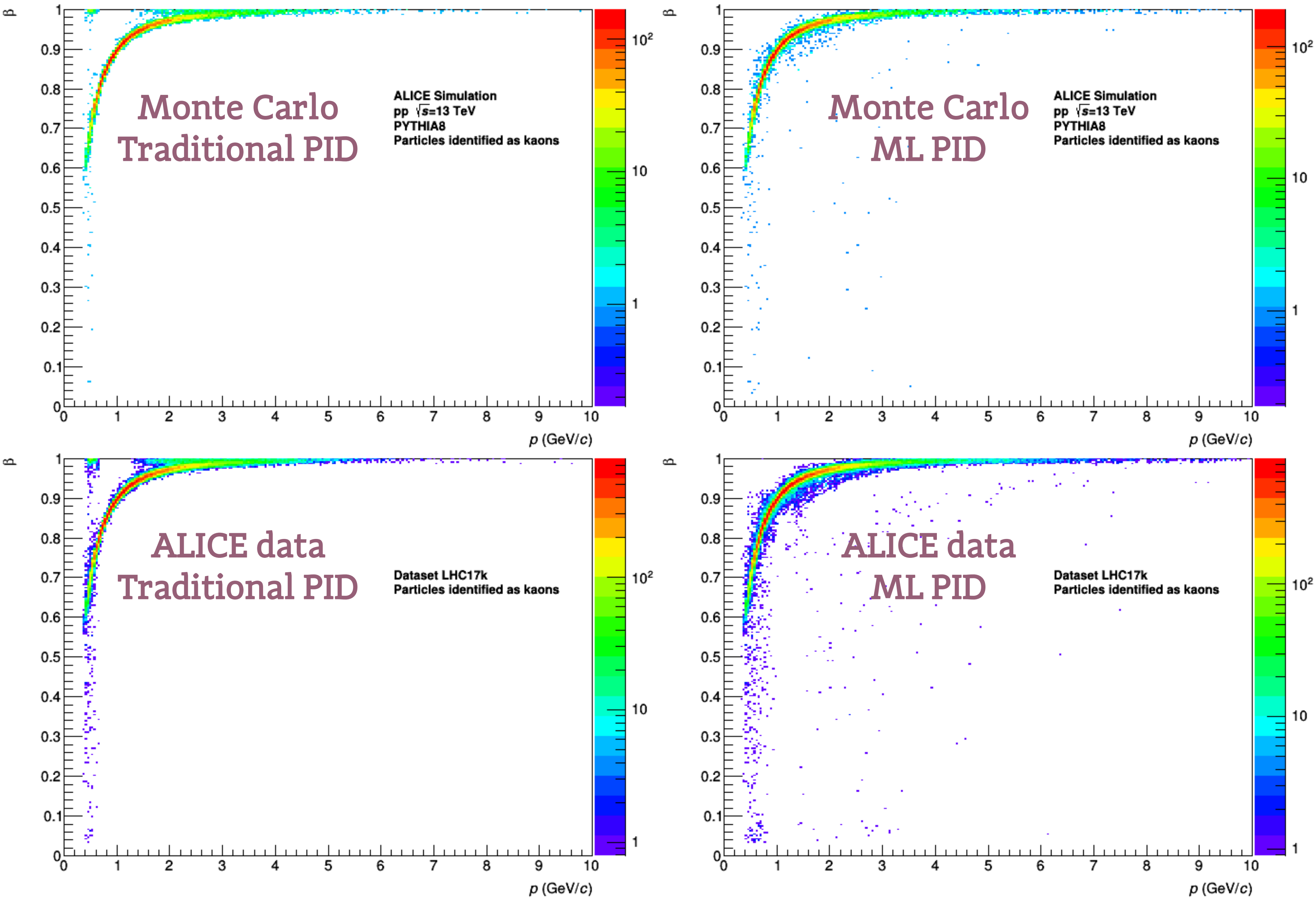


Summary

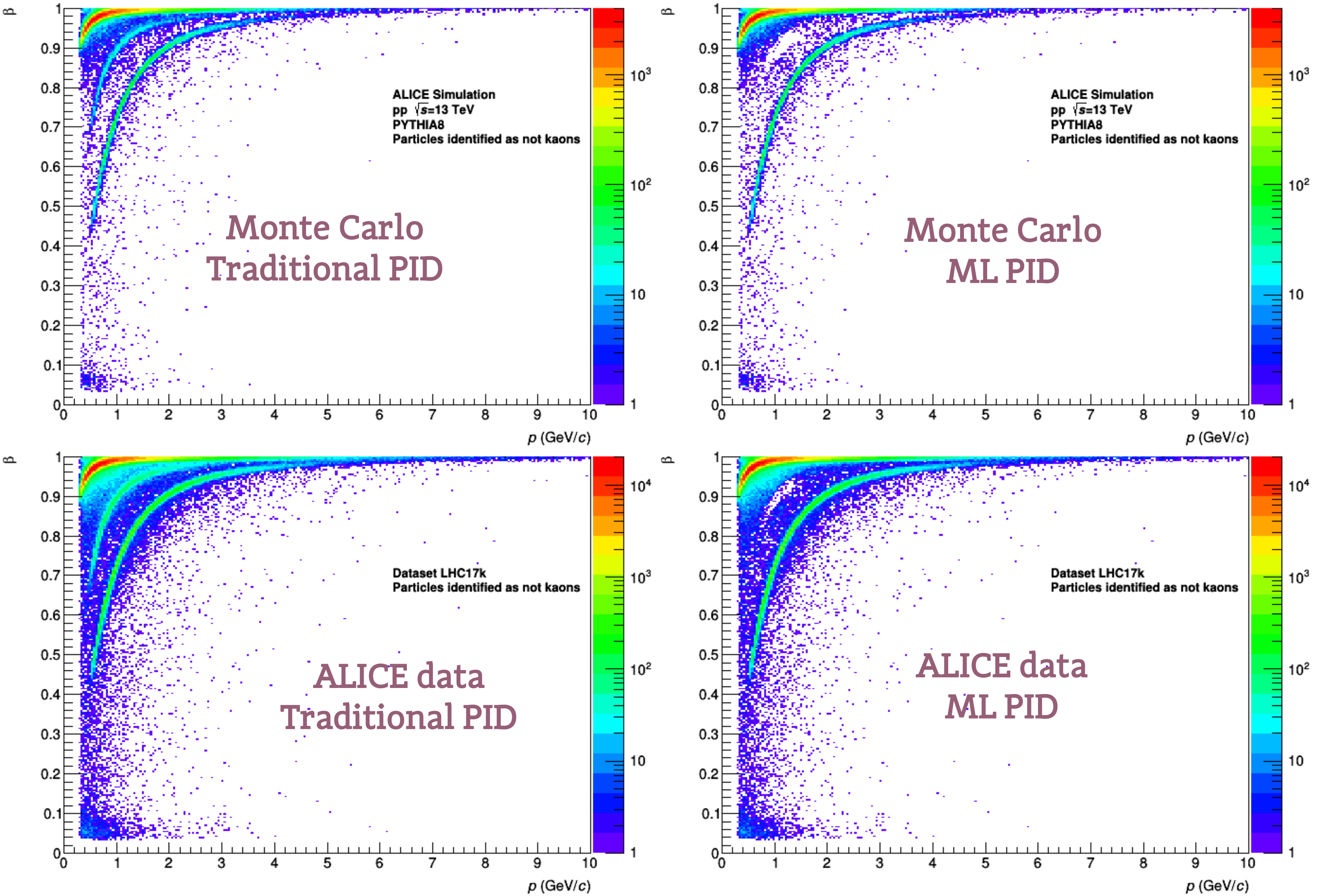
- ML-based PID outperforms traditional PID, especially in the low momentum region
- Training needed only once for each data set – no need for manual cut optimizations
- Quality of final classification more vulnerable to discrepancies between MC and real data
- Domain Adaptation techniques look very promising → hope to deliver working interface in O^2
- **Problems encountered in preliminary work:**
  - track-by-track implementation in AliRoot (optimal from our side) is very slow
  - C++ <-> Python connection is also a weak point

Backup

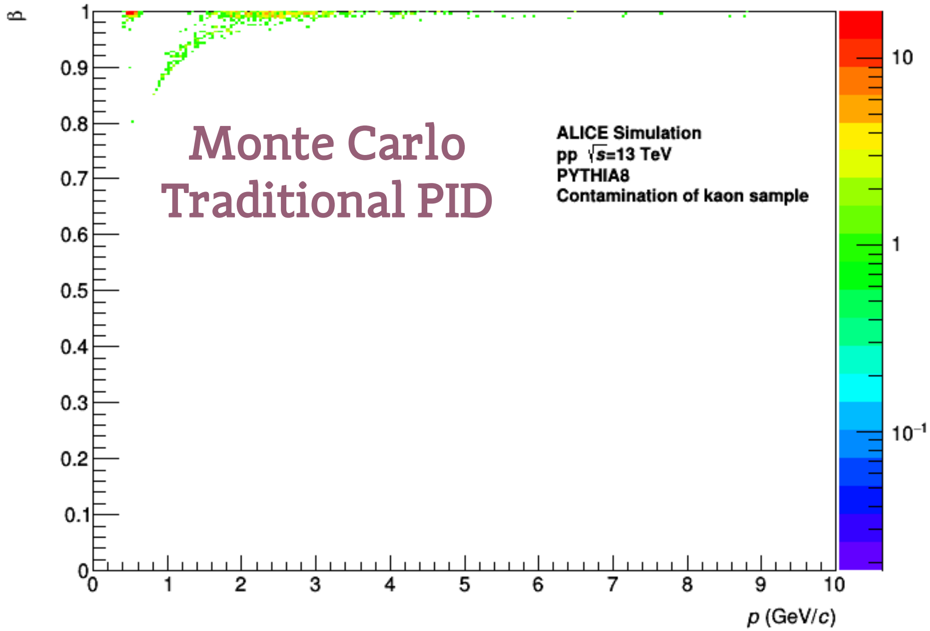
TOF accepted kaons

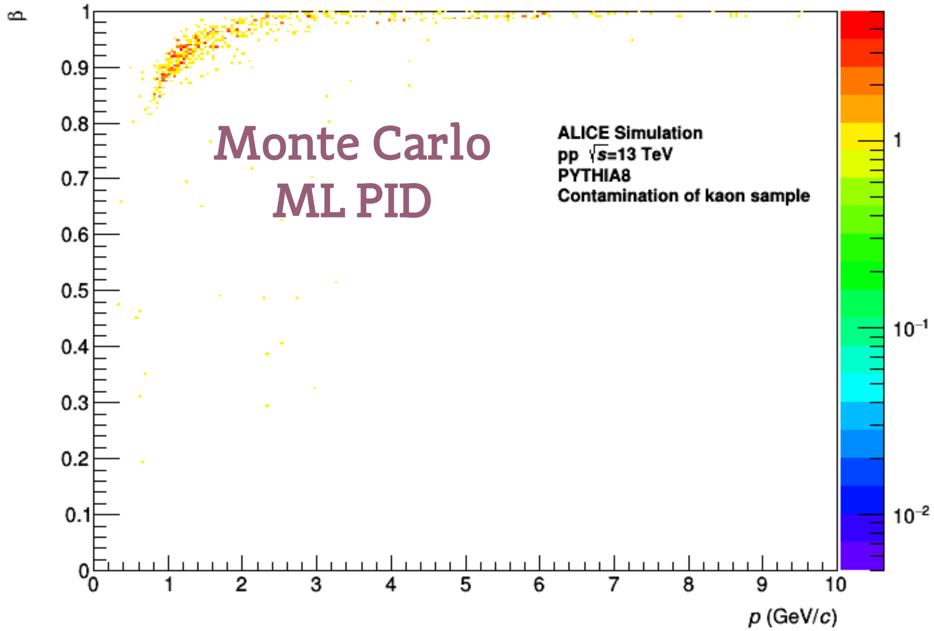


TOF rejected (not kaons)



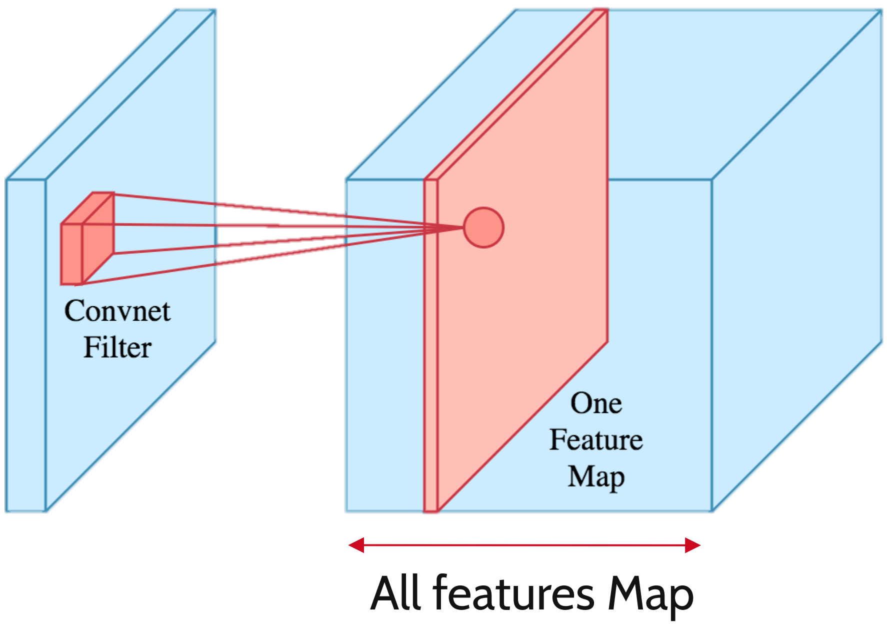
TOF contamination in kaons





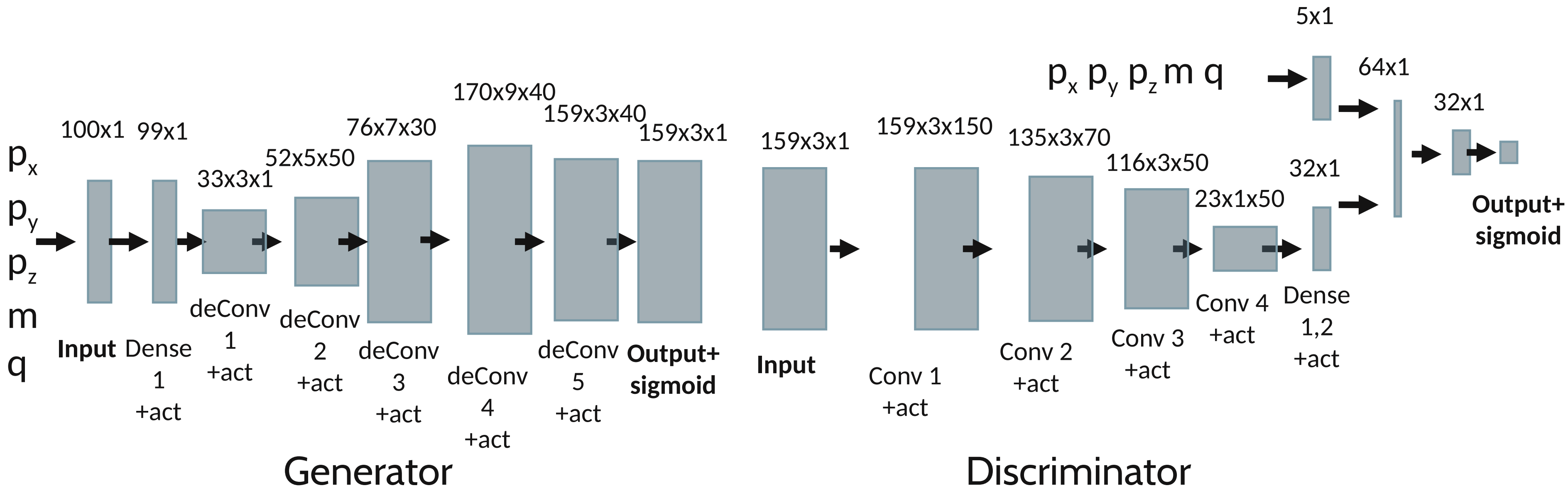
Deep Convolutional GAN

- Class of architectures which use the convolutional tools and deconvolutional layers – mostly used with images



condDCGAN: Conditional DCGAN

- Generator – deconvolutional layers
- Discriminator – convolutional layers
- Network conditioned on particle momenta, mass, and charge
- Output classification – sigmoid function



condDCGAN+: combined loss

- Training on on the full MC simulations
- Preparing the noise from initial parameters of MC simulations
- Comparing the generated samples with original ones
- Combining origininal conditional GAN loss with the results of comparison

$$\mathcal{L}_G(m, X) = \mathbb{E}_{z \sim p_z(z|m)}[\alpha \log(1 - D(G(z))) + \beta \frac{1}{n} \sum_{i=1}^{n} (X_i - G(\hat{z})_i)^2]$$

m - initial parameters (particle momenta),
X - original value corresponding to m ,
p(z|m) - distribution of a noise vector under initial parameters m
z - input into a generator
G and D - generator and discriminator
n - the number of produced clusters

Additional parameters α and β are used to weight the share of individual losses.
Best performing values are α = 0.6 and β = 0.8

Other areas of research

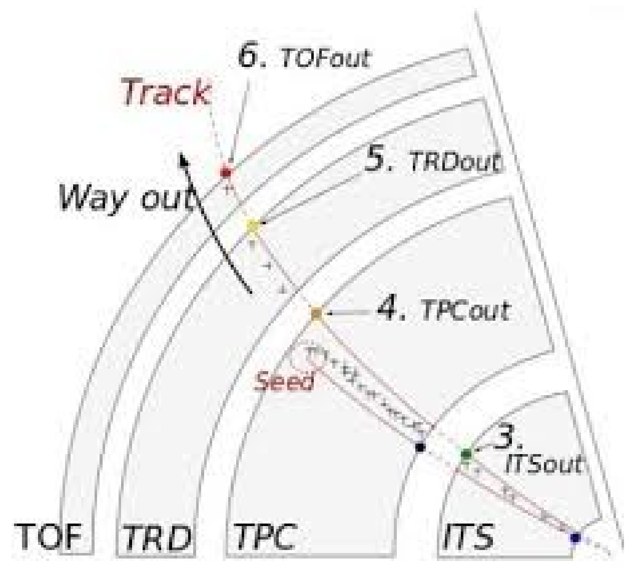
- Data Quality Assurance – prediction of detector quality label assignment

- Simulation of TPC clusters in Monte Carlo data using generative networks
  → next slides

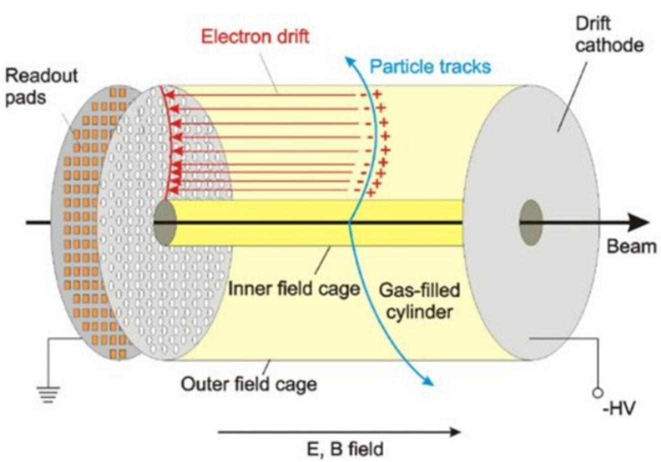
Simulation of TPC clusters in Monte Carlo data using generative networks

Time Projection Chamber

- Tracking in ALICE is performed by ITS, TPC, TRD and TOF
- First attempts – focus on the TPC only:
  - main tracking device
  - located from 0.8 m (inner radius) to 2.5 m (outer radius) from the beam and extending ~2.5 m in each direction along the beam axis
  - volume of 95 m^3
  - filled with Ne-CO_2 gas mixture (90%-10%)
  - **clusters** - points in 3D space, together with the energy loss, which were presumably generated by a particle traveling through
  - provides up to 159 clusters per track



ALICE Data Preparation Group



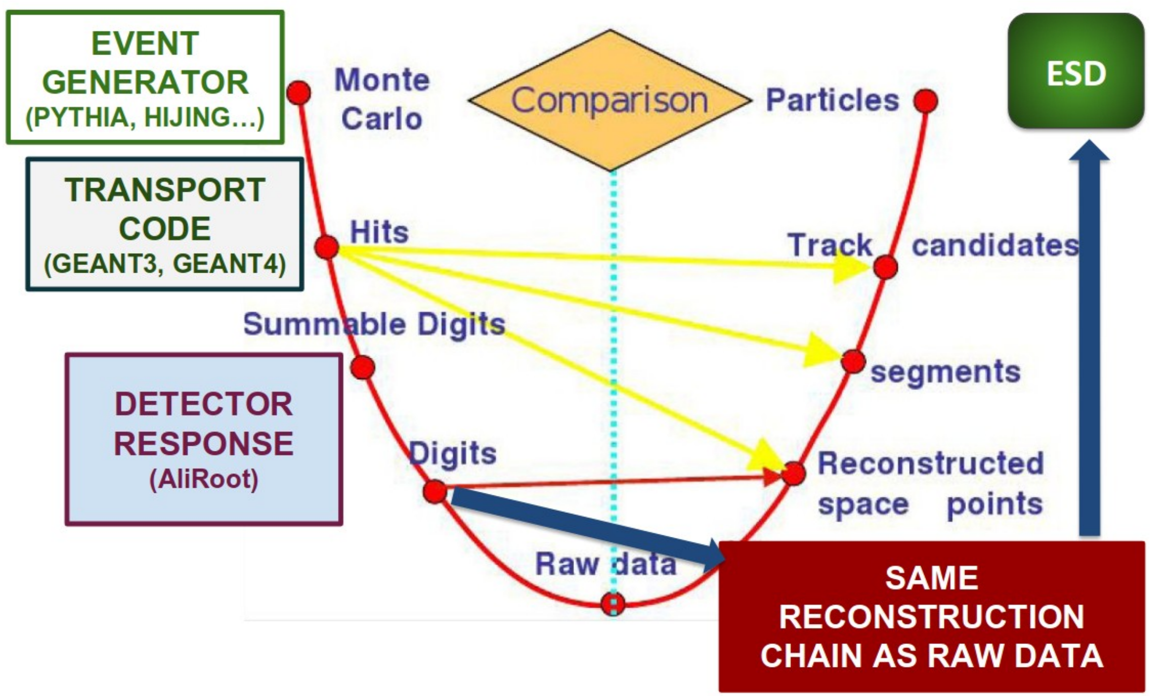
I.Konorov, Front-end electronics for Time Projection chamber

Simulation and reconstruction

- Current process relies on 5 independent modules
- The computationally most expensive module is particle propagation through the detector's matter

Collision generator → Particle propagation → Electronic signals (digits) → Digits to Clusters → Tracking

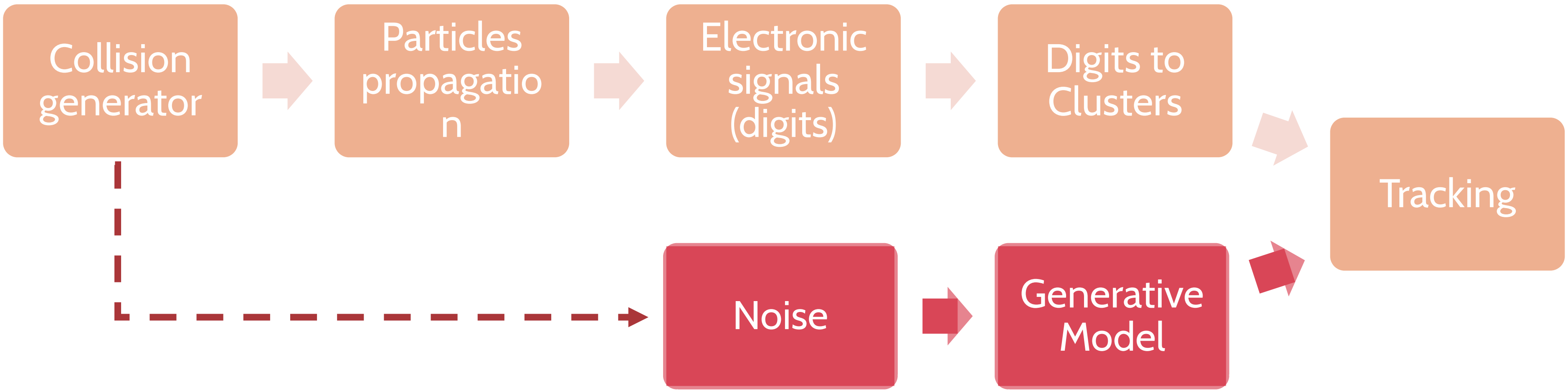
Monte Carlo simulation



Real data

ALICE Data Preparation Group

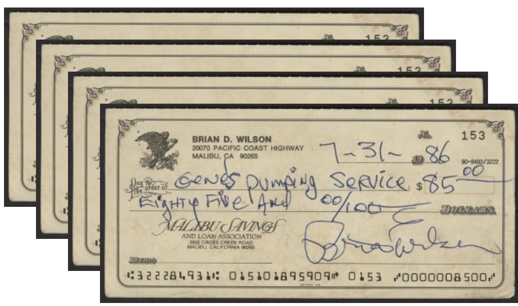
Simulation and reconstruction



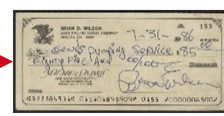
- **Generative solution for cluster simulation:**
  - substitute the detector simulation and check for the speed-up
  - full simulation **still needed** to generate training samples
  - **immediate drawback:** quality of such MC data can be either comparable or lower than the full detector simulation – limits potential applications

Generative Adversarial Networks

- Generative Adversarial Network (GAN) is a neural network architecture of two networks competing with each other (playing a min-max game)
  - **"Generator"** is trained to produce fake data resembling the real data
  - **"Discriminator"** aims to predict whether an example data is real or fake



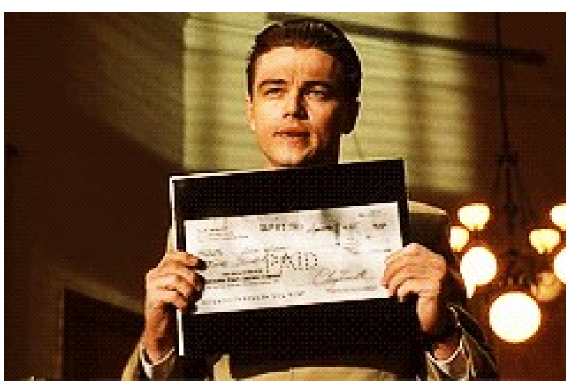
https://33milesinnewaygocounty.files.wordpress.com

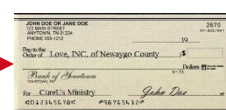


Discriminator

https://thechive.files.wordpress.com

Generator



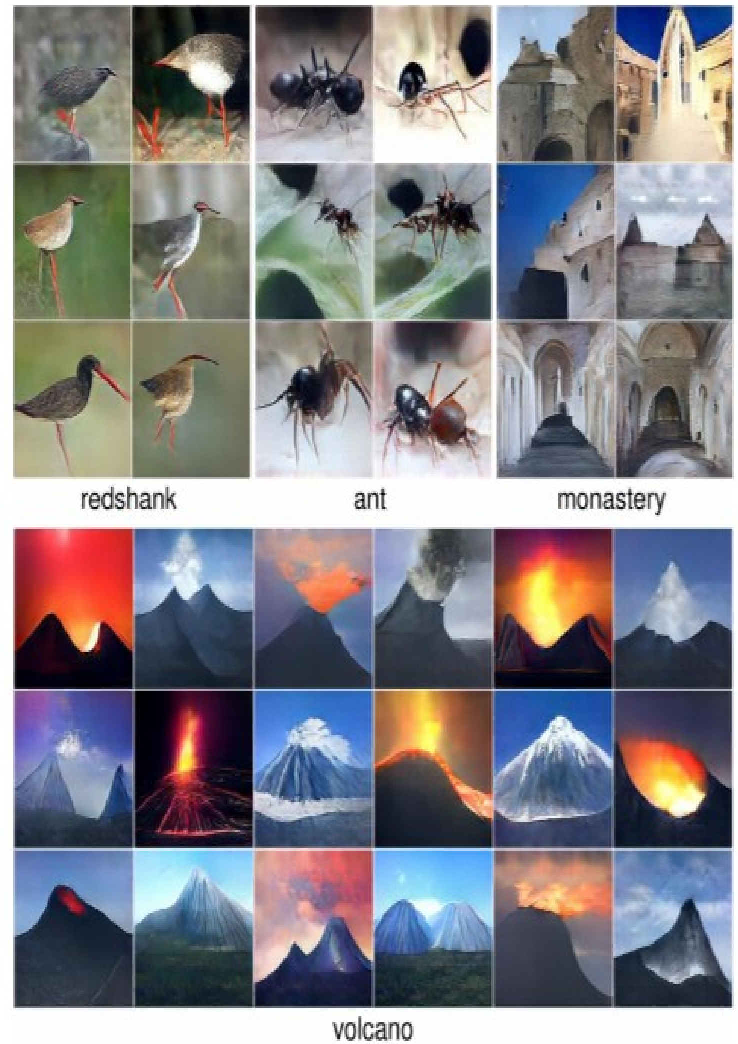


https://giphy.com/gifs/leonardo-dicaprio-catch-me-if-you-can-5leocharacters-t1h4nnWEWKfn2

Generative Adversarial Networks

- Typical use cases:
  - mainly generation of photo quality fake images (i.e. of celebrities)

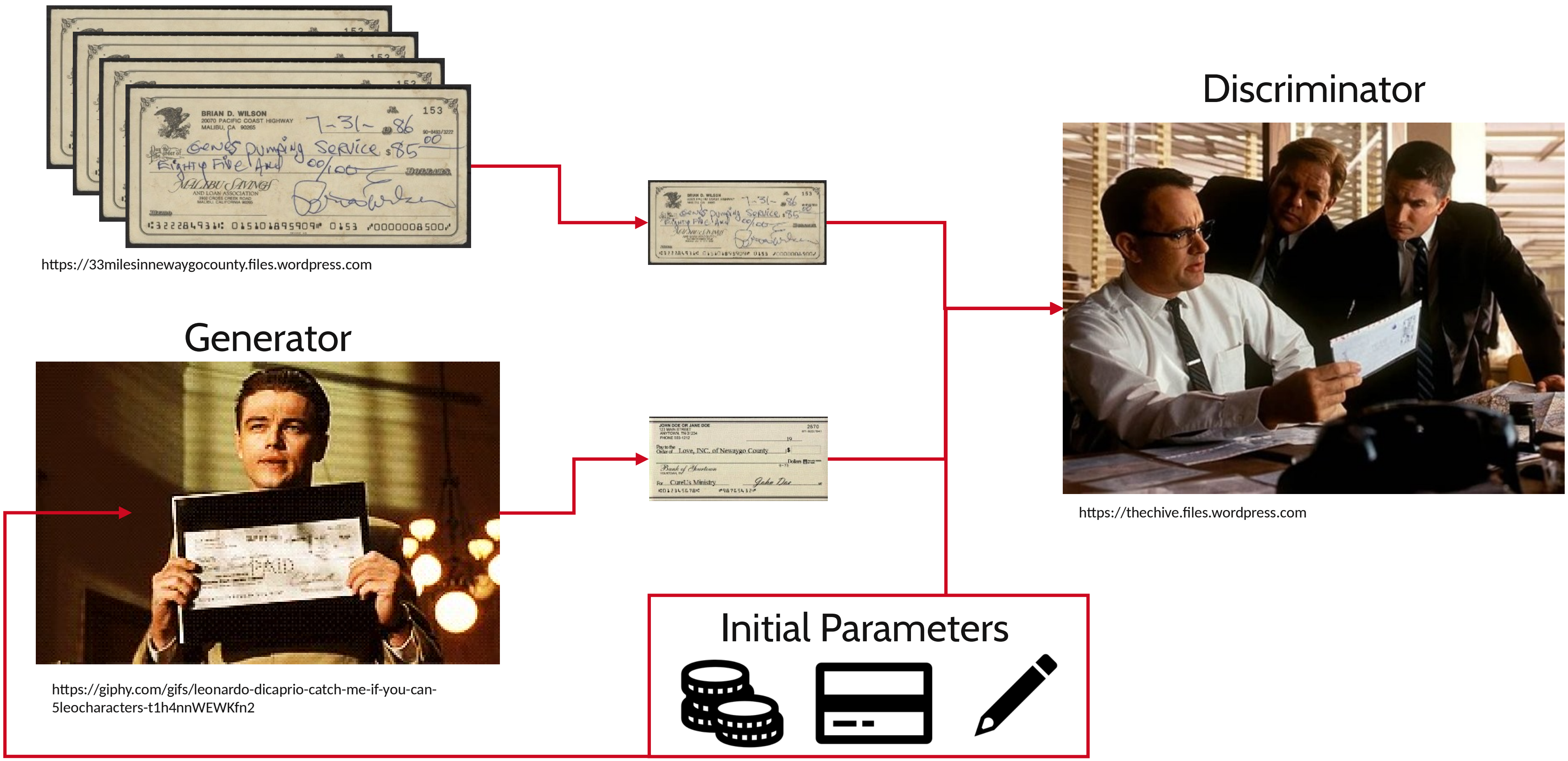
https://arxiv.org/abs/1710.10196



https://arxiv.org/pdf/1612.00005v1.pdf

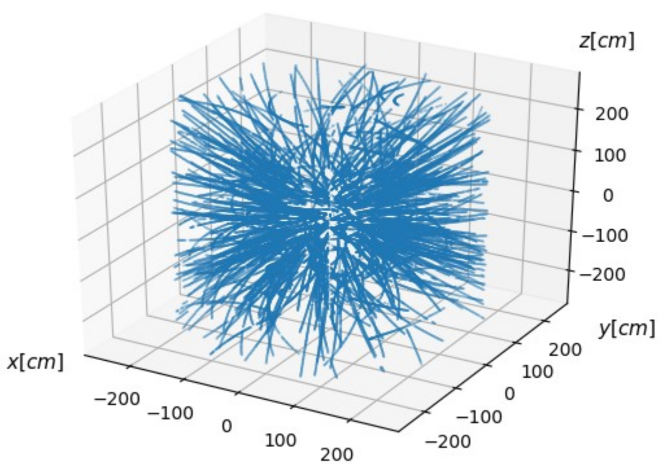
Generative Adversarial Networks

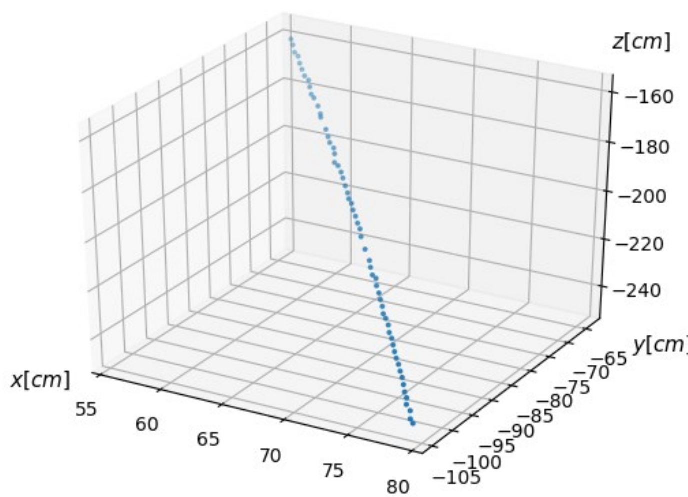
- **Extending the GAN architecture – provide a set of initial parameters for the generator and discriminator:**
  - generator would not generate a random output, but a customized one
  - in our case: initial momenta of Monte Carlo particles



TPC clusters with GANs

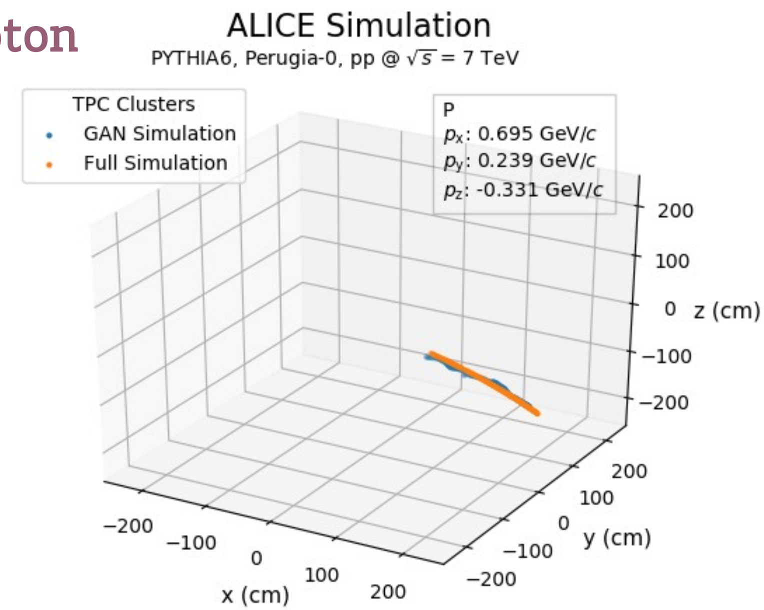
- It is not (yet!) possible to generate the full 3D image of the event at once (especially in the Pb-Pb event)
- Our solution is to:
  - generate clusters for single particles
  - two separate flows for spatial coordinates (x,y,z) and the energy
  - in the beginning focus only on 3D coordinates
  - merge generated samples (individual particles) into full images
  - training of the GAN on original full simulations



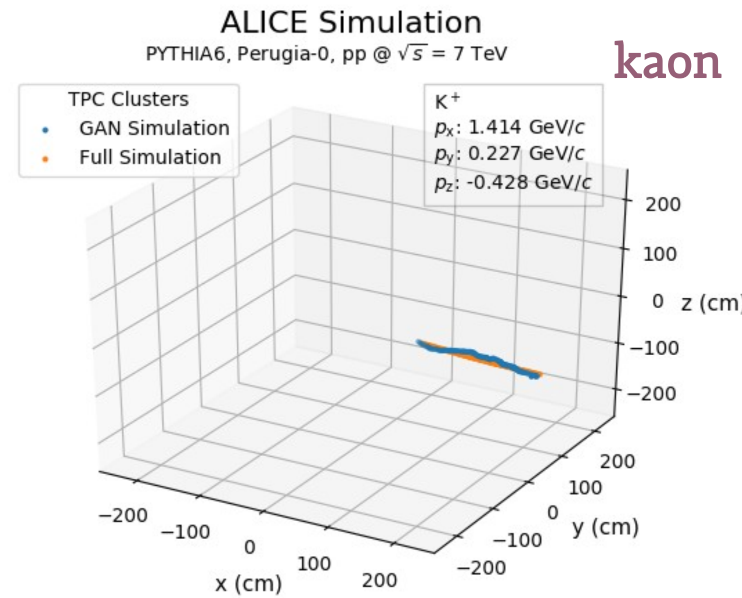


Example results

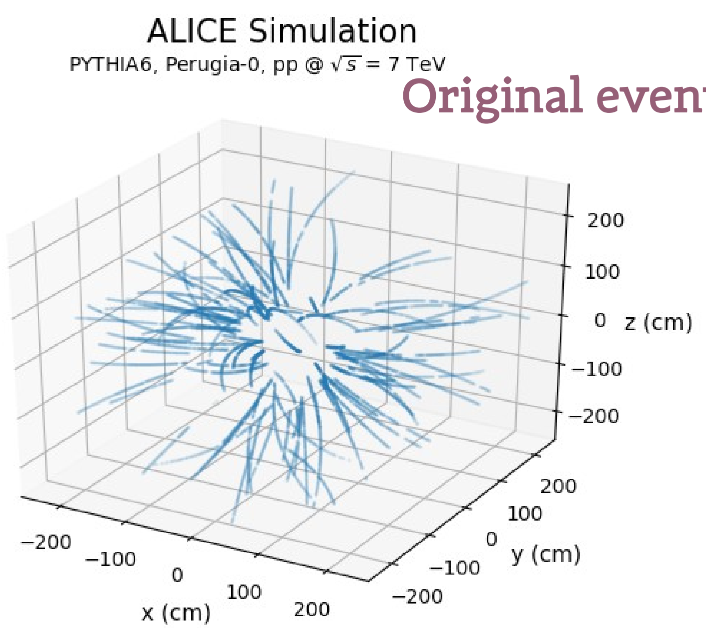
proton



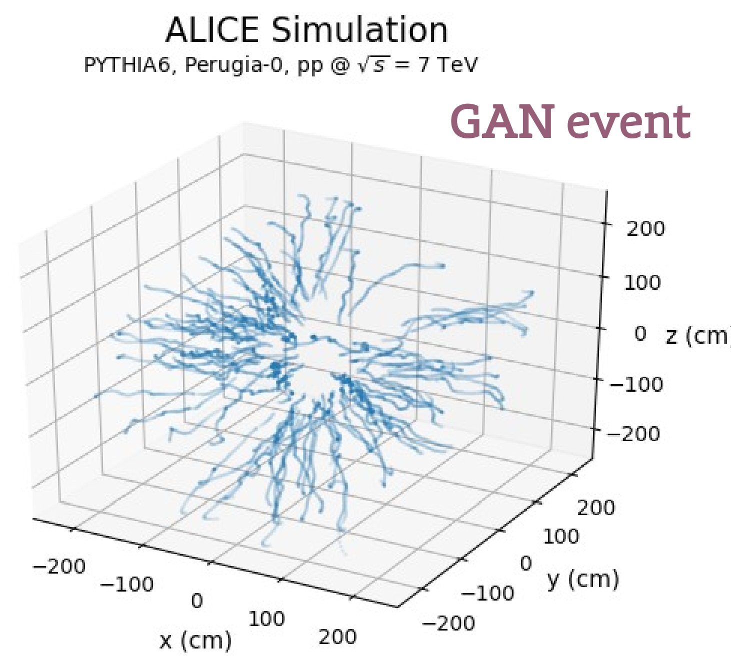
kaon



Original event



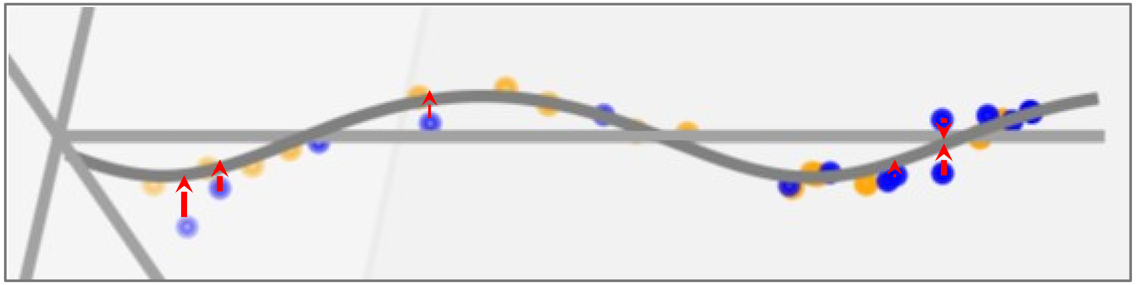
GAN event



Results

- Mean Squared Error (MSE) from the original helix as a quality measure
- Evaluation conducted on the separate test-set with ~15000 tracks

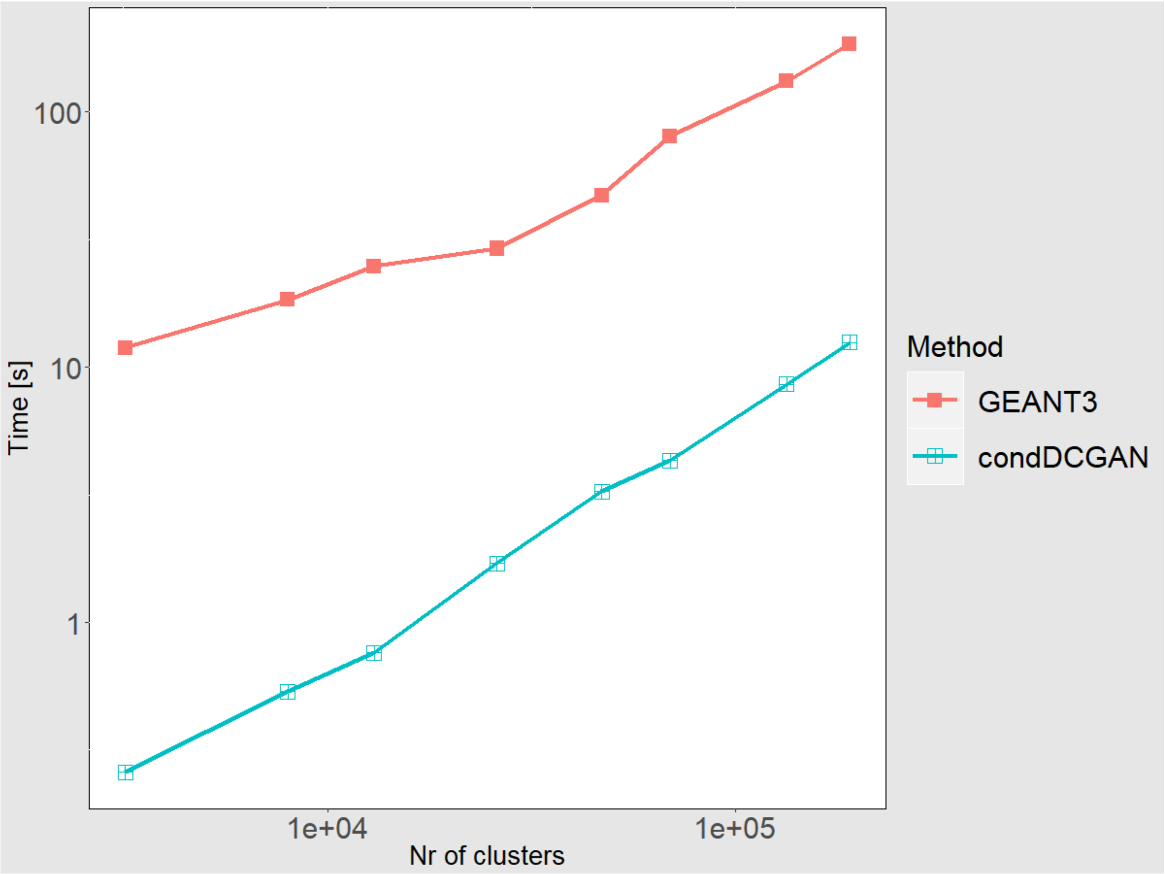
MSE visualisation:
Red - error
Grey- ideal helix
Orange – original clusters
Blue – generated clusters



Method	Mean MSE (mm)	Median MSE (mm)	Speed-up
GEANT3	1.20	1.12	1
Random (estimated)	2500	2500	N/A
condLSTM GAN	2093.69	2070.32	100
condLSTM GAN+	221.78	190.17	
condDCGAN	795.08	738.71	25
condDCGAN+	**136.84**	**82.72**	

Computational cost

- Performance test conducted on the standalone machine with Intel Core i7-6850K (3.60 GHz) CPU using single core and no GPU
- Additional order of magnitude speed-up for GAN models with nVidia Titan Xp GPU



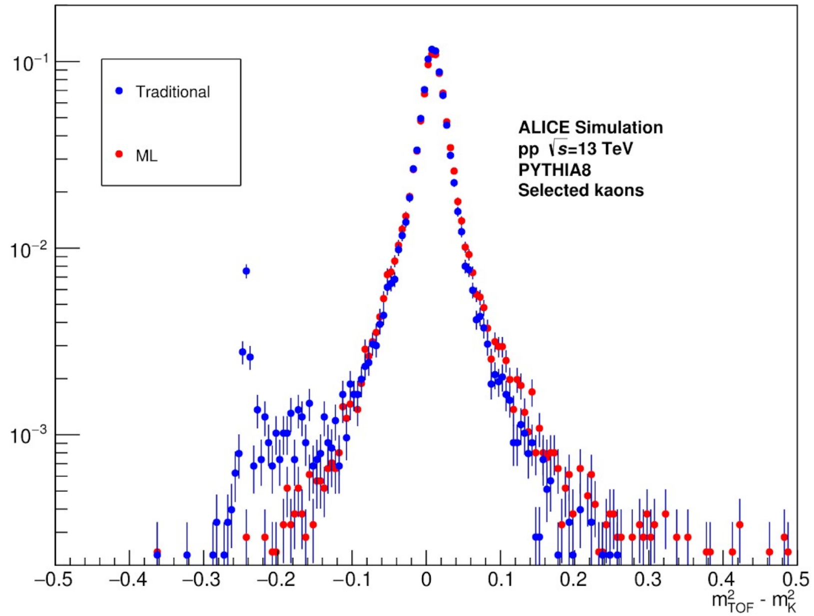
TOF time

- From our point of view TOF has a fantastic feature of a possibility to calculate mass of the recorded particle and compare it to the one from PDG

$$m_{TOF}^2 = p^2\left(\frac{1}{\beta} - 1\right)$$

- Thanks to that we can test contamination independently of MC simulations

Monte Carlo



ALICE data